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García Martínez, A.; Monsalve-Serrano, J.; Martínez-Boggio, SD.; Roso, VR.; Souza Alvarenga Santos, ND. (2020). Potential of bio-ethanol in different advanced combustion modes for hybrid passenger vehicles. *Renewable Energy*. 150:58-77.
<https://doi.org/10.1016/j.renene.2019.12.102>



The final publication is available at

<https://doi.org/10.1016/j.renene.2019.12.102>

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Additional Information

Potential of bio-ethanol in different advanced combustion modes for hybrid passenger vehicles

Renewable Energy

Volume 150, May 2020, Pages 58-77

<https://doi.org/10.1016/j.renene.2019.12.102>

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Abstract

The strong new restrictions in the vehicle CO₂ emissions together with the instability of the fossil fuels reserves reinforces the necessity to continue developing high efficiency combustion engines that operate with renewable energy sources. Bio-ethanol appears as a potential fuel to replace well-established fossil fuels, such as gasoline, due to the overall carbon neutral emission. In addition, the high-octane number allows to increase the compression ratio of the engine to improve the thermal efficiency. Apart from the CO₂, the emissions legislation restricts the NO_x and particle matter emissions to ultra-low values, and they will continue decreasing down to almost zero. In this work, two advanced dual-fuel combustion modes using bio-ethanol as main fuel are studied. A pre-chamber ignition system (PCIS) using bio-ethanol and hydrogen, and a reactivity-controlled compression ignition (RCCI) combustion mode operating with bio-ethanol/diesel was selected due to the potential to reduce NO_x emissions. These combustion technologies were studied by a numerical 0-D vehicle simulations in homologation and real-life driving cycles for a range extender hybrid powertrain. As a baseline, the original manufacturer spark ignition (SI) no-hybrid powertrain fueled with pure bio-ethanol was used. The powertrain components and control system were optimized to obtain the maximum overall vehicle efficiency, and low CO₂-NO_x emissions. Finally, a life cycle analysis (LCA) was performed to study the global potential of the bio-ethanol to reduce greenhouse gas (GHG) emissions. A battery electric vehicle (BEV) and a gasoline SI no-hybrid vehicle were added for comparison. The results show that the RCCI mode presents the highest potential to reduce the NO_x emissions. However, the PCIS allows to reduce the tank to wheel CO₂ emissions up to 60 g/km when high rates of H₂ are used. The LCA-GHG for the vehicles using bio-ethanol is 50% and 95% lower than a BEV and SI-gasoline vehicle, respectively.

Keywords

Pre-chamber, RCCI, Bio-ethanol, Hybrid powertrain, Emissions regulations, Driving cycles

1. Introduction

In the effort to control the global warming and fossil carbon emissions, many countries are proposing new policies to make their energy matrix more renewable [1]. The increase of the bio-ethanol use as a transportation fuel emerges as a short-term solution. The main reasons are the maturity of the production process and the possibility to be blended with gasoline, which reduces the total carbon content in the mix [2]. Moreover, the biogenic effect of using a renewable energy like the bio-ethanol helps in the reduction of total CO₂ emissions. The EU and other governmental authorities announce the necessity to cut the GHG emissions (mainly CO₂) in 2050 by 80% compared to 1990 levels [3]. Therefore, the monoculture of petroleum-based transportation must change if the target wants to be reached [4]. As a first step, it is necessary to improve the fuel production process as well as the infrastructure to have low cost and simple accessibility fuels for vehicle customers. In a second step, it is also necessary that the automobile sector advance in new combustion modes and more efficiently powertrains to allow finally the required ultra-low GHG emissions [5].

At present, the two major biofuels produced worldwide are bio-ethanol, from fermentation of sugars primarily in corn starch (USA) and sugarcane (Brazil) [6], and biodiesel from transesterification of vegetable oils, with bio-ethanol accounting for the majority of current biofuel production [7]. The GHG emission reduction potential of bio-ethanol, especially the cellulosic bio-ethanol, is recognized in the policies that address the reduction of the GHG emissions from the transportation sector [8]. Nowadays, the United States and Brazil, account for 85% of the worldwide bio-ethanol production [9]. Therefore, one main problem for the worldwide bio-ethanol use is the concentration of the production in a few countries. Other problem is that almost all the bio-ethanol around the world is produced directly or competing from food crops. This way of production is called first bio-ethanol generation (1GE). Therefore, other crucial task is the contention of fuel versus food that generate several debates around the world. Over the long term, the greatest potential for bio-ethanol production lies in the use of cellulosic feedstocks, which include dedicated energy crops and forest residues. Studies have shown that if 50% of the bagasse produced could be converted into bio-ethanol, it would represent improved production of 60% more liters per hectare [10]. This attractive possibility has put the second bio-ethanol generation (2GE) to the forefront in the global agenda towards the advanced biofuels [11]. Nonetheless, the cost and technological feasibility remain major barriers to such commercial production [12]. These problems and concerns have directed the search for the third bio-ethanol generation (3GE) feedstock from marine algae. The integration of algae as a sustainable feedstock for bio-ethanol has gained worldwide attention in terms of food security and environmental impact [13]. From a research and development perspective, there have unquestionably been advances in the main scientific and technological fields related to biofuels and bio-ethanol; however, from a production perspective, this is not so evident. In spite of the mentioned challenges, the gradual substitution of fossil by bio-based fuels seems to be the first step to reach the GHG emissions goals and achieve a more renewable energy mix.

The use of renewable low carbon fuels directly impacts in the CO₂ emissions of the transportation sector. However, to achieve a real reduction of all emissions it is necessary to technologically improve the combustion process and powertrains efficiency. In this line, the advanced combustion modes appear as a potential option to

improve the internal combustion engines (ICE) efficiency and emissions (NO_x , Soot, HC, CO, etc) [14]. The use of lean mixtures with high exhaust gas recirculation rates or stratified distribution in the main combustion chamber have presented good results in the past [15]. The lower average temperatures and the oxygen excess from the lean combustion decreases the heat losses to the cylinder walls and also reduces the formation of undesired pollutant emissions such as NO_x and soot. However, there are significant challenges regarding combustion control and stability, initial kernel development and flame propagation speed [16]. The PCIS is an option to improve the well establish SI system when lean air-fuel mixtures are used [16,17]. The active pre-chambers use a supplementary fuel in a small volume outside of the main combustion chamber with high turbulent intensity to start the combustion process. This pre-chamber is connected to the main combustion chamber (similar used in SI system) through a series of small orifices. Therefore, there is an ejection of hot gases from the pre-chamber to the main chamber allowing multiple ignition locations for the lean air-fuel mixture presence in the main chamber. Fuel as hydrogen (H_2) [18] and methane (CH_4) [19] were already tested in lean gasoline-, ethanol-, methane-air lean mixtures with benefits mainly in fuel consumption and NO_x emissions.

Other line of investigation in advanced combustion modes are the use of low temperature combustion (LTC) modes in compression ignition (CI) engines as the RCCI combustion. In this concept, two fuels are injected into the cylinder using separated injector systems. Thus, the quantity of each fuel can be varied independently depending on the engine operating conditions. A low reactivity fuel (LRF) is injected in the intake port using a port fuel injector (PFI) and a high reactivity fuel (HRF) is injected using a direct injector (DI). To achieve a highly efficient RCCI operation with low emissions, the major part of the total injected fuel should be LRF (gasoline, ethanol, methanol,...), while the HRF (diesel) is used to trigger the combustion process and promote a reactivity stratification inside the cylinder [20]. It shows great advantages in terms of combustion control and NO_x -soot reduction without thermal efficiency losses [21]. In spite of the benefits in terms of emissions of the abovementioned combustion modes, the thermal efficiency gains are low (below 3%) [22]. Therefore, to achieve better results in terms of overall vehicle efficiency, the electrification of the powertrain appears in the last few years as a reliable technology to be applied in commercial vehicles [23]. The main advantages of the powertrain electrification are the possibility to make a more intelligent energy use and the recovery of the brake energy due to a high-power battery package and the presence of an electric motor (EM) coupled to the wheels [24]. The position of the EM defines the hybrid electric vehicle architecture. The series, or also called range extender, has an EM coupled to the wheels (traction motor-TM) and other motor (generator-GEN) coupled to the internal combustion engine (ICE) to recharge the batteries. The range extender architecture emerges as solution to improve the electric range of battery electric vehicles (BEV) and solve the lack of recharge electric stations without increasing the battery package [25].

All these technologies show great potential to reduce the GHG. However, to compare the real benefits of different transport solutions is necessary to see the overall process. In this line, the life cycle analysis (LCA) is used by several researchers to analyze the impact of different technologies [26,27]. Specifically, in the LCA modeling of a vehicle, the foreground system (production, use phase, and end-of-life treatment) can be differentiated from a background system (materials, resources, electricity,

infrastructure provision, and waste generation) [28]. This allows to identify the main harmful components and the potential points to be improved. Nowadays there are available several databases as: GREET, Gabi, BioenergieDat, etc., which contain information of each item in terms of emissions and resources use. By means of an LCA for bio-ethanol, Daylan et al. [6] showed that one kilometer driven with a E85 fueled vehicle (85% bio-ethanol and 15% gasoline) could reduce the GHG emissions by 47% and ozone layer depletion emissions by 66%, relative to a similar pure gasoline fueled vehicle. Therefore, the use of bio-ethanol as a substitute for fossil fuels like gasoline seems to have great potential to reduce the GHG emissions.

In spite of the different advantages of these technologies shows by the authors in the abovementioned works, up to the knowledge of the authors, only exist a few works combines advanced combustion modes and hybrid powertrains in transient conditions [24,29]. In addition, there is none publish works that compare the potential of bio-ethanol as main fuel in PCIS and RCCI. Thus, the aim of this work is the study of the performance and emissions of a passenger car with the use of bio-ethanol as main fuel in advanced combustion modes when the powertrain has a conventional layout (no hybrid) and a range extender hybrid technology. These results are compared with a bio-ethanol fueled SI ICE in the conventional and range extender hybrid version. Both powertrains are compared at the same maximum power output level, the additional electrical component weight are added to the original vehicle weight and homologation and real-life driving cycles are used for comparison. The vehicle fuel economy and emissions determined by a numerical OD vehicle model, feed with experimental engine test bed results, is further incorporated into the Argonne National Laboratory's Greenhouse gas, Regulated Emissions, and Energy use in Transportation (GREET®) model [30]. The LCA considers the GHG emissions and energy use associated with the production of the bio-ethanol in Brazil and USA for different feedstocks. A BEV and a pure gasoline SI vehicle are considered in the LCA as reference for the comparison. Thus, the results of this work will contribute to understand the benefits of advanced combustion modes in hybrid powertrains and add novelty information with respect to vehicle fuel consumption and emissions. This last point is strongly important to annually reports that evaluate all the new technologies in the transport sector.

2. Materials and Methods

The evaluation of the range extender series hybrid vehicle with the use of three combustion modes (SI, PCIS and RCCI) was performed in a numerical 0-D vehicle model. The model was fed with experimental results obtained in two engine test beds to reproduce with accuracy the ICE behavior. After the performance and emissions results were obtained, a numerical LCA model was used to evaluate the impact of each technology in an overall perspective. The modeling procedure and the methodology to post process the results are explained in the next subsections.

2.1. Vehicle Numerical Model

The vehicle behavior was modeled by a 0D-powertrain code developed in the GT-Suite interface (v2019, Gamma Technologies, LLC., Westmont, IL, USA) [31]. The software includes several modules that allow the study the vehicle behavior in transient conditions. The speed-time profile (driving cycle) is inserted in the driver module.

Therefore, the model is capable to calculate the vehicle traction forces in the wheels considering the road friction and aerodynamic forces, among others. This signal it is received by the vehicle controller and a response it is sent to the ICE, electric motors and brakes. For the energy management, a rule-based controller (RBC) was used due to the robustness and low computational costs [24]. Deterministic rule-based controllers use a set of rules to determines the action over the components as ICE, EM and batteries. This is implemented using a state machine or supervisory controller.

The vehicle selected to perform the simulation is a passenger car Class B (Ford Fiesta), which equips the SI engine used in one of the experimental test benches. The main parameters of the vehicle are described in Table 1. This vehicle has a conventional powertrain architecture (no-hybrid) with the ICE coupled to a manual 5-gear transmission by a clutch. The final coupling is done by the differential with the front wheels. This original equipment manufacturer (OEM) powertrain layout was used as baseline case to the comparison with the hybrid powertrains.

Table 1 - Vehicle specifications.

Vehicle type [-]	Passenger class B
Base vehicle Mass [kg]	1145
Passenger and Cargo Mass [kg]	145
Vehicle Drag Coefficient [-]	0.33
Frontal Area [m ²]	2.04
Tires Size [mm/%/inch]	180/60/R15
Differential ratio [-]	3.5
Transmission ratios [-]	3.8/2.0/1.3/1.0/0.7



The electrification of the powertrain was performed by the addition of electric motors and a high-power battery package in the numerical models. In spite of several powertrain layouts were designed along the last years (P0, P1, P2, Power Split, etc), the series or range extender emerge as a solution to improve the efficiency of ICE at low speed and loads [32]. In addition, this layout reduces the transitory behavior of the ICE. Figure 1 shows a scheme of the proposed powertrain layout. The ICE is separated of the wheels and coupled to an EM dedicated to operate as a generator. The wheels are propelled by another EM (traction motor-TM) coupled by the traditional differential system. The battery package is fed by the generator when the ICE is turned on, and gives the necessary energy to the TM to follow the driving cycle required. Other capacity of this type of vehicle is the brake energy recovery by the TM and storage in the battery package. This enables the use of an additionally energy that improves the global efficiency of the vehicle.

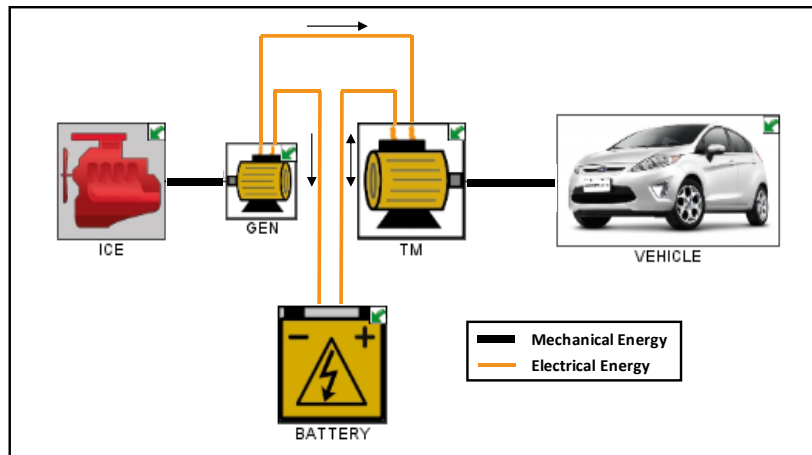


Figure 1 – Series Hybrid Powertrain Layout

To be comparable the hybrid vehicles with the no-hybrid case, the same maximum power output was used (90 kW). Therefore, the traction motor of the range extender concept was modeled as an electric motor with a constant power of 90 kW between 0-6000 RPM. This power curve against motor speed is characteristic of the interior permanent magnet electric motors [23]. The generator was also kept constant at 30 kW due to approximately the maximum achievable power of the advanced combustion modes (PCIS and RCCI). The battery capacity was optimized in the range between 2-12 kWh, typical range of full hybrid vehicles [33]. The battery voltage was set around 400 V. A variation with the state of the charge as well as the internal resistance was implemented to model the behavior between charge and discharge cycles. All the weight corresponding to the added electric components was added to the OEM vehicle weight. The average bibliography values were used, with 0.4 kg/kW for the electric motors and 10 kg/kWh of battery capacity [23]. In spite of the low recharge available power (ICE-GEN max power), these type of concepts were already used by Mahle [34] and Nissan [35] in class B passenger cars. The main reasons are the possibility to use a low power rate ICE, medium size battery package (strongly lower battery requirements than a BEV or PHEV) and avoid the addition of a transmission. In terms of components size and vehicle packaging, fast improvements were seen in the last years to allow the use of this range extender FHEV technology in small and medium cars. Minimizing the package and weight of the engine and electric motors were deemed to be of paramount importance to maximize the applications that the range extender unit would fit into. As Figure 2a shows, the integration of the generator and traction motor to the ICE is crucial to be able to be applied in commercial small passenger cars. In general, the battery package is included in the rear of the vehicle in a similar layout to the liquid fuel tank (see Figure 2b).

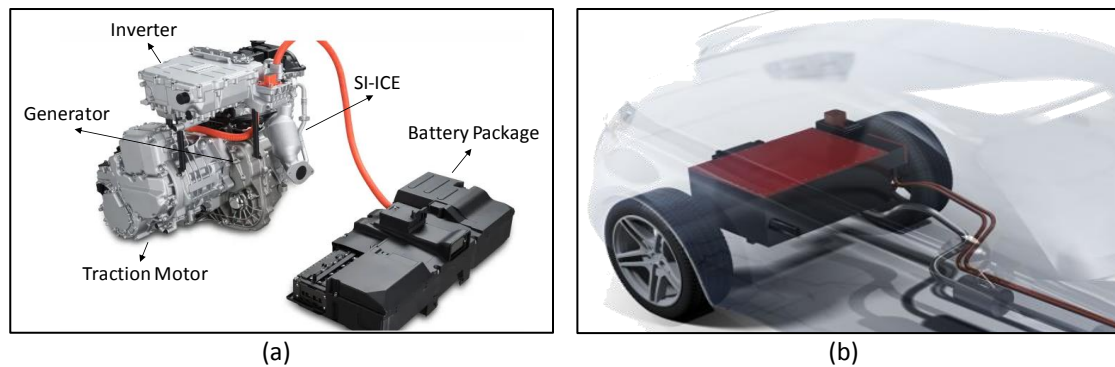


Figure 2 – Range extender components (extracted from Nissan Leaf class B passenger vehicle [35]) (a) and battery package location (extracted from Audi A1 class B passenger vehicle [34]) (b).

As abovementioned, the supervisory control of the vehicle was carried on according to a series of rules (RBC system). For the range extender, the main parameter is the battery state of charge (SOC). In a previous work, the authors analyzed the effect of different initial levels of SOC and charge levels in a similar vehicle setup but with a RCCI diesel-gasoline ICE calibration [36]. Between 2 and 3 levels of power charge was concluded to be the best configuration. The initial SOC was not seen important in the final simulation results. In this work, as the range of ICE power for the advanced combustion mode is narrow (0-30 kW) than in a conventional pure gasoline or diesel calibration (0-90kW), 2 charge levels were preferred. In addition, the starting SOC was selected at a medium range (65%) with respect to the maximum battery energy.

Figure 3 shows a scheme of the battery SOC along a driving cycle. The vehicle operates in depleting mode (ICE off) until the first SOC level set at 58% was reached. When this battery charge level is reached, the ICE is turned-on and works in first level of power at stationary condition that it is optimized in a design of experiments (DoE). If the power level is not enough to reach the initial SOC and continues decreasing until 50% (1550 s at Figure 3), the ICE will change to the second charge level (maximum available power) to recovery the battery charge until the driving cycle ends. The example shown in Figure 3 uses the ICE 3 times in the level 1 of power and then changes from the level 1 to the level 2 one time to reach the initial SOC at the end of the cycle. This condition, equal SOC_{final} and $SOC_{initial}$, is mandatory in the WLTP to be comparable with traditional no-hybrid vehicles. The optimization procedure was performed by a DoE in which 800 different battery capacity and operational points were tested by the discretization with a Latin-hypercube statistic selection. See previous work of the research group [33] for more information in the optimization methodology.

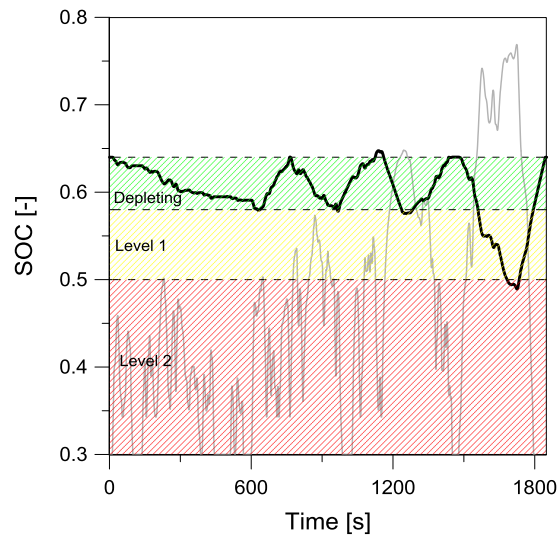


Figure 3 – Example of the SOC behavior and charge level states in a WLTC.

The vehicle fuel consumption and emissions were tested under the WLTC that is a driving cycle that aims to represent a typical travel of any person around the world. In addition, it is used in the currently in force protocol to measure the emissions and fuel consumption for homologating the passenger cars in Europe (WLTP) [37] but it was developed intending to be a standard to be adopted by most of the countries. As shown in Figure 4a, the WLTC has four different zones called low, medium, high and extra-high. The first two are representative of urban driving and the last two are representative of rural and highway areas, respectively. The protocol includes hybrid electric vehicles inside the test. For no-plug in hybrid vehicles the laws are similar to those for no-hybrid cars, with the main constrain being that the HEV at the end of the cycle must have the same battery SOC that was set at the beginning of the test.

In addition to the WLTC, other three driving cycles were used to analyze the performance of the different vehicles under real-life conditions. These cycles were measured by the authors with a GPS-data logger in Spain and Brazil. Figure 4b shows an urban cycle of 10 minutes and top speed of 40 km/h, representative of a heavy traffic condition. Figure 4c is a combined cycle with a first 13 minutes of urban area and then the transition to a rural area for approximately 16 minutes. Lastly, Figure 4d is a pure highway driving cycle in which 270 km are travelled in around 2.4 hours. The top speed in these two last cycles is over 120 km/h to represent real drive conditions.

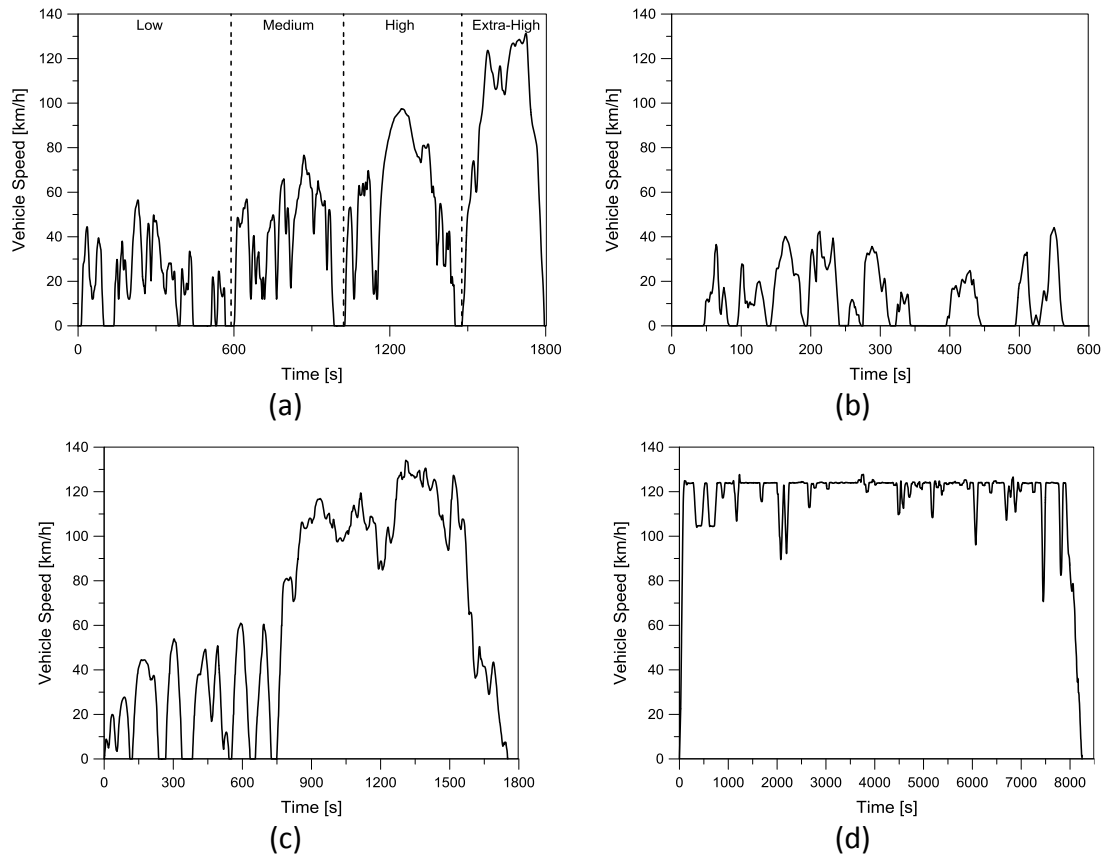


Figure 4 – Driving cycles to test the vehicle behavior in transient conditions: WLTC-Homologation cycle (a), Urban (b), Combined (c) and Highway (d).

In terms of emission regulations, there is not a clear agreement to fix a level of NO_x , CO, HC, particle matter (PM) and number (PN) among all the countries. The European Union (EU) regulate the emissions by means of the Euro 6, defining a limit value per vehicle category and the WLTC as the main vehicle test cycle. However, this normative use different emissions levels for compression ignition and spark ignition engine. As the Euro 6 emissions limits can be simply taken as reference for a particular vehicle knowing the power to mass rate, these limits were used in this work. In spite of other criteria and levels could be adopted (Tier 3-USA, LEV III-California), the purpose of using these values is only for comparison. Table 2 shows the values taken for the different emissions.

Additionally, since 2009, the EU legislation sets mandatory CO_2 emissions reduction targets for new cars. Fees will be applied to the car manufacturers if the average CO_2 emissions of their fleet exceed the target in a given year. The target of 130 g/km was phased in between 2012 and 2015. A phase-in period will also apply to the target of 95 g/km. From 2021, the average emissions of all newly registered cars of a manufacturer will have to be below the target. The manufacturers are incentivized to put on the market zero- and low-emission cars, emitting less than 50 g/km, through a “super-credits” system. The main objective for 2030 is to reduce by 48% the CO_2 levels of 2015. The last European statistics results, from 2018, show that the car fleet average was already at 120 g/km. See Table 2 for more information of the CO_2 target levels.

Table 2 –Pollutant Emissions reference Euro 6 limits and EU CO₂ targets.

Parameter	Limit PI-PFI [g/km]	Limit CI [g/km]
CO	1.0	0.5
HC	0.068	0.09*
NO _x	0.06	0.08
PM	-	0.05
CO ₂ 2021 Target	95	
CO ₂ 2025 Target	80	
CO ₂ 2030 Target	67	
CO ₂ Taxes incentive	50	

2.2. Experimental Set Up

The main experimental inputs for the model calibration are the engine maps for fuel consumption and emissions obtained in stationary and warm conditions. This methodology was already used by the authors [38] and other researchers [39] with a good accuracy in transient conditions. The main assumption of the model is the quasi-stationary behavior of the ICE. In spite of that some instantaneous phenomena are not considered, the overall error is below 1% for the fuel consumption and 5% for the NO_x and soot emissions measured in a conventional diesel Euro 6 powertrain [38]. This error is acceptable when the objective is the comparison of different vehicle platforms and combustion modes in large driving cycle. The computational effort allows testing over 2 hours of driving data in a couple of minutes. In addition, as the range extender use pre-defined stationary point for a quite-long period (over 5 consecutives minutes), so the similarities to the map based approach will be closer than the previous test no-hybrid or P2 hybrid vehicles [38].

In this work two engine test bed were used to the study of three different combustion modes. As the main target of this work is the use of bio-ethanol in different combustion technologies to study the advantages and drawbacks, all the combustion modes have the ethanol as main fuel (higher proportion in mass basis than the secondary fuel). For comparison purpose, the baseline case was a commercially SI-PFI ICE fueled with hydrous ethanol. A SI engine was selected as reference due to the current market trend in the European Union for this segment cars. This ICE was named as Engine 1 and in Table 3 the details are presented. The fuel-air mixture was fixed around the stoichiometric value ($\lambda=1.0$). This approach is the most used by car manufacturers due to due the possibilities of having a controlled combustion stability and to use a three-way catalyst (TWC) to reduce NO_x, CO and HC with the same aftertreatment system (ATS).

In a second step, the experimental tests were performed substituting the conventional SI system by the PCIS and adding a new line of fuel for the secondary fuel (H₂). The volume added with the pre-chamber was offset by a recess in the cylinder head. Therefore, the volumetric compression ratio from the baseline SI engine was not changed. Thus, the system now is composed by a pre-chamber and a main combustion chamber. This added pre-chamber has an internal volume of 0.88 cm³, representing 2.2% of the main combustion chamber volume. In addition, it has five interconnecting holes to the main combustion chamber, four of which have 1 mm of diameter and an angle of 45° versus the normal axe, and the remaining one is located at the center with a diameter of 2 mm. In this combustion mode, the ethanol is used as main fuel injected

in the PFI system and enters in the main chamber with the opening of the intake valve. As secondary fuel, hydrogen is injected in the pre-chamber. Therefore, the jet flames from the pre-chamber rapidly propagate in the main chamber and act as distributed ignition kernels. Thus, increases the turbulence and the mixing rate of the unburned mixture, providing more interaction between fuel and air molecules. In previous work, it was seen improvements in combustion initiation due to higher turbulence intensity and propagation speed of H₂ [18]. Also, the effect in the main combustion chamber temperature was minimum with respect to the lean SI case. All this effect promotes the combustion obtaining higher thermal efficiency and lower NO_x than the SI-ethanol stoichiometric case.

The RCCI-ethanol test was performed in a single-cylinder engine compression ignition original designed to operate with conventional diesel combustion (CDC). This engine is based on a serial production light-duty GM 1.9 L platform used in passenger vehicles. The piston used is the serial one, with a re-entrant bowl that confers a geometric compression ratio of 17.1:1. An additional PFI system was installed to inject the LRF (ethanol). As HRF a commercial diesel was used with the OEM system configuration, direct injector. For this engine, the values obtained in the SCE were scaled to the multi-cylinder engine without any variation. This hypothesis was already used by other authors with success [40].

Table 3 - Engine characteristics.

Parameter	Engine 1	Engine 2
Engine Type	4 stroke, 4 valves, Pre-chamber/PFI-SI	4 stroke, 4 valves, direct injection
Number of cylinders	4	4
Displaced volume	1596 cm ³	1910 cm ³
Stroke	81.4 mm	90.4 mm
Bore	79 mm	82 mm
Compression ratio	11.0:1	17.1:1
Rated power	90 kW@ 6000 rpm, Gasoline/ethanol	105 kW@ 4000 rpm, Diesel

As was described above, several fuels were used for the different combustion modes. However, the similarity between them is the ethanol as main fuel. Table 4 shows the fuel main properties of the four different fuels. The SI and PCIS systems use hydrous ethanol, which is largescale commercially available in Brazil. This fuel not contains gasoline in the mixture; Thus, in this work was called E100. The small percentage of water is due to residues of the distillation process. Gaseous hydrogen (H₂) is use in the pre-chamber for the ignition of the lean ethanol-air mixture. The high lower heating value (LHV) and propagation speed should improve the combustion process. In the case of the RCCI mode, a mix of ethanol and gasoline was used. The main reason is the ignition problem at load loads that occurs when pure ethanol is injected in the CI combustion chamber. Therefore, to promotes the combustion, 15% of gasoline in the ethanol is used (E85). The E85 is the highest ethanol fuel mixture found at largescale in the US and several European countries, particularly in Sweden. As Table 4 shows the use of H₂ and ethanol could allow the reduction of CO₂ production in the combustion process due to a reduction in the carbon content by 100% for H₂, 41% for E100, and 23% for E85 with respect to the diesel. It is important to note that for ethanol, the low LHV will increase the fuel consumption and the CO₂ emissions. Therefore, the best way to know if the use of ethanol effectively reduces the total GHG emissions is a driving cycle test.

Table 4 - Fuel used in the calibration maps main properties.

Parameter	E100	H ₂	E85	Diesel
Composition	96% Bio-ethanol / 4% Water	Hydrogen	85% Bio-ethanol / 15% Gasoline	Diesel (EN590)
LHV [MJ/kg]	25.5	120.0	31.6	42.5
Density [kg/m ³] @ 300K, 1atm	799	0.08	784	842
RON	>100	>130	108	-
MON	92	-	89	-
Cetane Number	-	-	-	51
AFR _{stoichiometric} [kg/kg]	8.4	34.2	9.8	14.5
CO ₂ /Fuel Ratio [kg/kg]	1.87	0	2.43	3.17

The calibration of the advanced combustion mode has as main targets the reduction of pollutant emissions without losing thermal efficiency. However, one of the hardest points in the calibration of light duty vehicles is that the homologation procedure not restricted in terms of brake specific emissions (g/kWh) as in medium- and heavy-duty engines. On the contrary, the limit is set depending on the emission mass per kilometer (g/km). Therefore, this work evaluates by numerical models if the calibration is enough to achieve the required emissions values and the final fuel/energy consumption.

For the PCIS E100-H₂ mode an interactive strategy between the injection timing, injection duration and ignition timing parameters were performed to achieve an optimized condition during the engine calibration. The injection timing was calibrated to achieve the lowest coefficient of variation of IMEP (CoV_{IMEP}). The minimum acceptable limit was set at 5% due to previous experimental and bibliography results [41]. The injection duration was adjusted to maintain the desired global lambda. The global air-fuel mixture ratio was set at $\lambda=1.4$, to achieve an extend engine operation map in lean condition. Lastly, the ignition timing was tuning to obtain the maximum brake torque without knocking events. The hydrogen injection was increased until achieving the lowest possible CoV_{IMEP}, being the fuel burned in pre-chamber a mixture of ethanol that enters from the main chamber in the compression process and the directly hydrogen injected. It is important to note that any change in one of these parameters interferes in the others, being a loop calibration. It was finished when any benefits in terms of fuel consumption and emissions is seen. The tests were conducted at an engine speed range varying from 1000 rpm to 3000 rpm in steps of 250 rpm, and five different accelerator positions from 0% to 100%. More information about the engine calibration procedure is explained in [18].

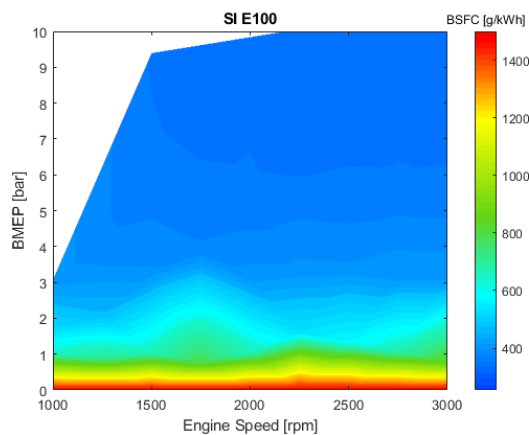
The RCCI E85-Diesel dual fuel mode engine calibration map was reached by means of three consecutive steps. The starting point was to set the parameters similar to the conventional diesel combustion (CDC) calibration. Then, diesel energy was change by E85 energy to reduce the combustion chamber temperature and NO_x. The stable combustion was achieved (coefficient of variation, CoV_{IMEP} < 5%) through the ethanol mass fraction and diesel start of injection (SOI) modification without exceeding the mechanical limits (maximum in-cylinder pressure among others). In addition, the EGR rate is also tuned to reduce the NO_x and soot emissions levels up to extreme low values, maintaining the combustion stability. At the same time, ethanol fraction and diesel SOI are readjusted to improve the performance-emissions trade-off at this point. The last step consists of refining slightly the calibration in terms of EGR and diesel SOI to try to

reduce the unburned products and the fuel consumption without exceeding the rest of the limitations. Additional information about the engine calibration procedure is explained in [42].

The total brake specific fuel mass consumption (BSFC) in the stationary maps for the three combustion modes are showed in Figure 5. For the three cases the fuel consumption improves with the engine load. The PCIS shows advantages in the low load zone of the map with respect to the SI case. Also, the RCCI case shows better behavior than the SI in this load zone, mainly attributed to the more efficiently combustion seen in CI diesel engines. The minimum BSFC was achieved for the RCCI (255 g/kWh), then the PCIS (325 g/kWh) and finally the SI (334 g/kWh).

In terms of brake thermal efficiency, Figure A1 in the appendix shows a similarity between the SI and RCCI at the highest efficiency point around 42%. For the SI, this value was achieved at the highest engine speed and load tested (3000 rpm and 10 bar BMEP). In the case of the CI engine, the RCCI mode achieved the best combustion operation at medium engine speed and medium load (2000 rpm and 6.5 bar BMEP). This is explained because at this operating condition, the RCCI mode could be better tuned due to the lower in-cylinder pressure peaks than at higher load and engine speed. Lastly, the PCIS shows an inverse trend in brake thermal efficiency than that seen in BSFC when compared to the SI ethanol. This is explained by the fact that the hydrogen has 5 times higher LHV than the E100 (Table 4). Therefore, when the fuel consumption is compared on energy instead of mass basis the PCIS has lower benefits than the SI concept. In spite of this point, the renewable source of hydrogen and its zero-carbon content could improve the results in terms of CO₂ emissions and fuel cost.

Figure 6 shows the percentage of ethanol mass in both dual fuel combustion modes. For SI this proportion is 100%. The PCIS uses in the range of 95-100% of ethanol meanwhile the RCCI is noticeably smaller (45-75%). Above 2 bars of BMEP in the RCCI mode, the ethanol fraction is minimum due to high rates of CO and HC.



(a)

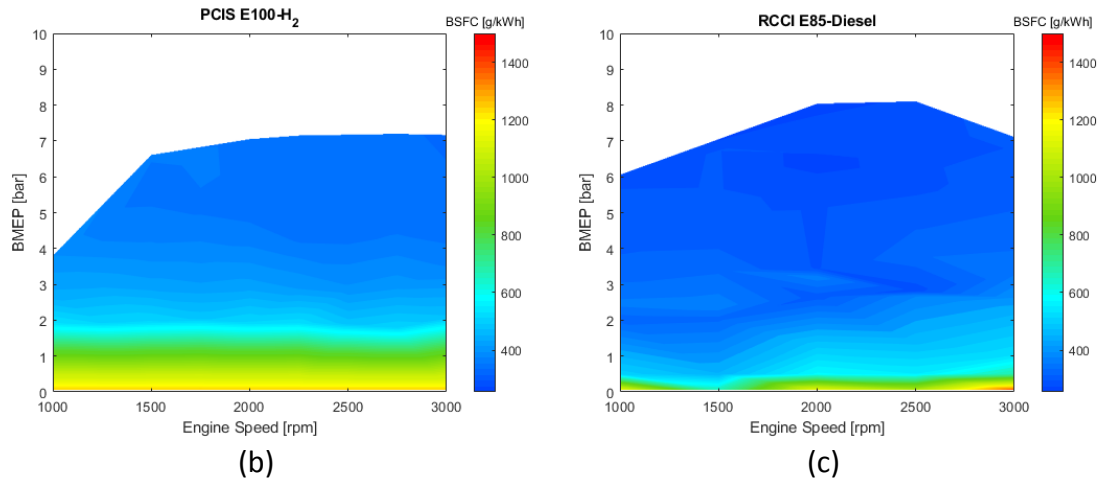


Figure 5 – Brake specific total fuel consumption for SI E100 (a), PCIS E100-H₂ (b) and RCCI E85-Diesel (c).

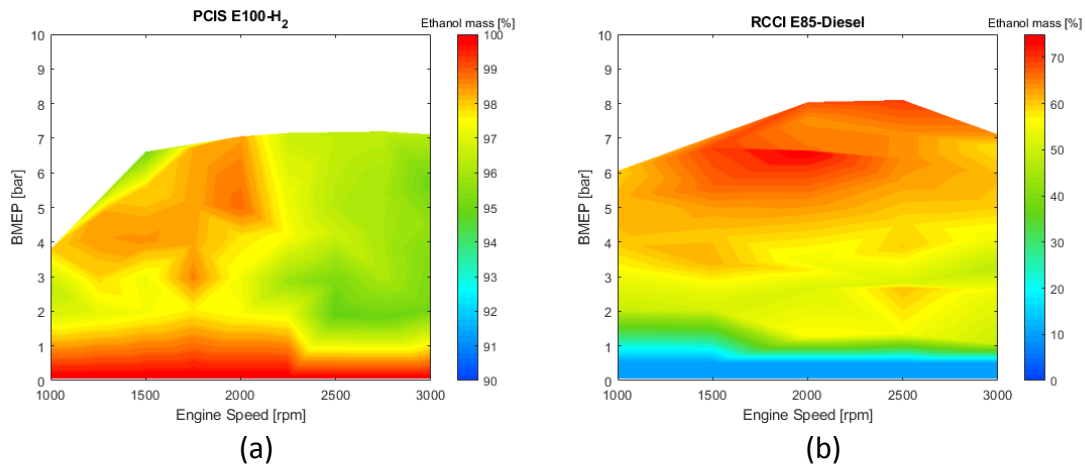


Figure 6 – Ethanol mass percentage over the total fuel mass injected for PCIS E100-H₂ (a) and RCCI E85-Diesel (b).

As mentioned previously, the use of the PCIS and RCCI mode instead of SI and CDC is mainly to reduce NO_x emissions. Figure 7 shows the standard spark ignited and the two advanced combustion modes engine-out NO_x. The NO_x reduction is evident with PCIS map using Engine 1 (same than SI system) all below 1.7 g/kWh and an average value of 0.9 g/kWh. The stoichiometric calibration, with the SI system, achieve 10.7 g/kWh with an average value of 5.5 g/kWh. In the case of the RCCI, the NO_x emissions are even lower with a maximum value of 0.7 g/kWh and average of 0.4 g/kWh. To determine if these values attend the actual emissions legislation, transient vehicle test must be conducted. This is one of the objectives of the present work, through numerical modelling by a 0D numerical model presented in the previous section.

In addition, the soot emissions present a strong decrease in the RCCI mode. For the SI-PFI and PCIS-PFI mode the particle emissions are negligible due to the homogeneous mixture between the fuel and the air [43]. This is the main reason why these last types of technologies do not need the use of particle filter as CI engines or DISI gasoline engines. Also, PFI engines are not restricted by normative. The Soot map it is included in the appendix at Figure A3 for brevity of the manuscript.

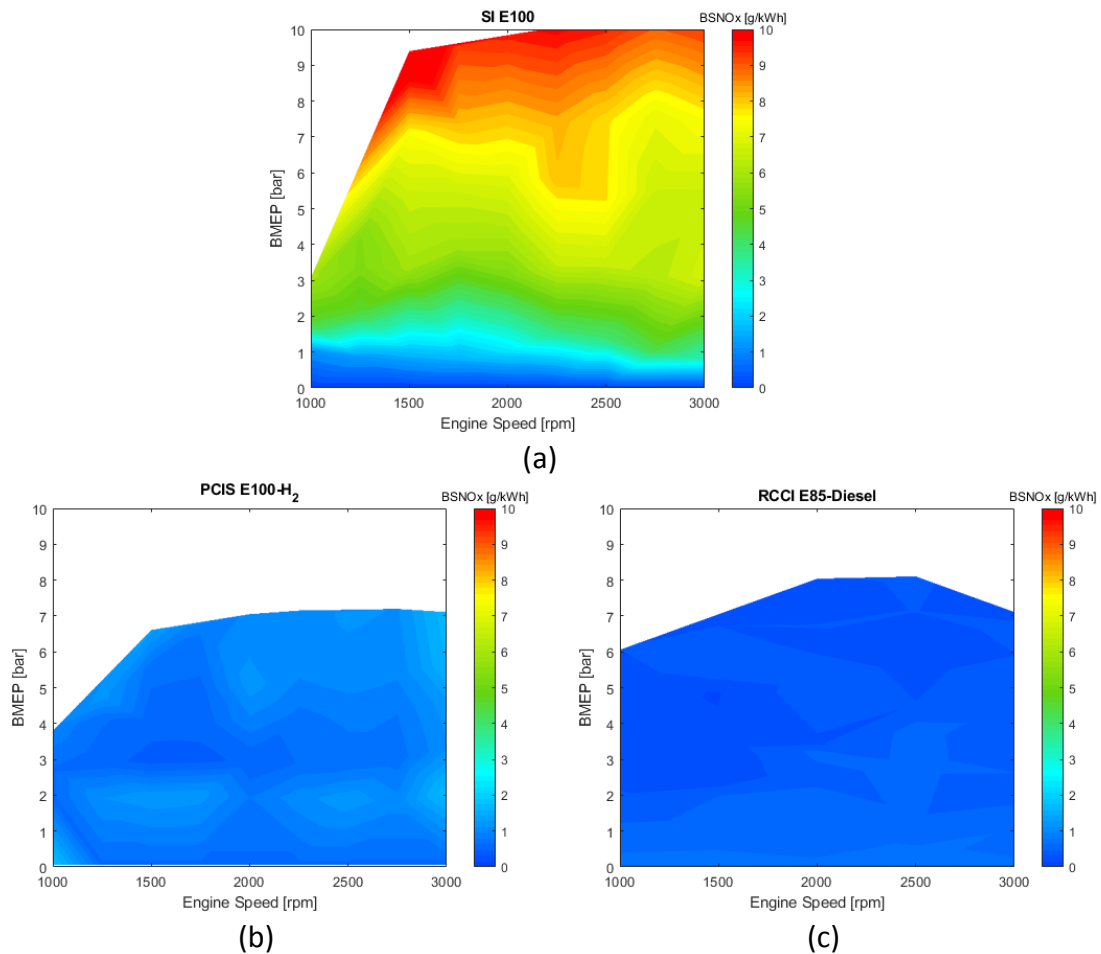


Figure 7 – Brake specific NO_x emissions at engine-out for SI E100 (a), PCIS E100-H₂ (b) and RCCI E85-Diesel (c).

2.3. Life Cycle Analysis Model

The Argonne National Laboratory created an open software to perform LCA on different passenger vehicles platforms called GREET [30]. It is a model widely used for analysis of life-cycle energy and environmental impacts of alternative and new transportation fuels and advanced vehicle technologies. It has become one of the essential tools used by researchers and policy makers in the US and abroad to evaluate different vehicle technologies. Also, EU has suggested to include in future legislation amendment to complement CO₂ TTW restrictions.

The carbon dioxide (CO₂), methane (CH₄), and nitrous oxide (N₂O) produced in different stages of the vehicle life are considered in terms of GHG emissions, and their global warming potentials (GWP, 100-year perspective). Approaches as gate-to-gate or cradle-to-gate and cradle-to-grave are usually used depends on the scope of the analysis [44]. As in this work an overall view of the vehicle life is sought, cradle-to-grave analysis was performed. This means that the analysis must to include material extraction and fabrication of the vehicle components, vehicle used (tank-to-wheel, TTW) and maintenance. In addition, the fuel production (well-to-tank, WTT) and the recycling of the vehicle in the end of life need to be added. A scheme of the different parameters added in the analysis is depicted at Figure 8.



Figure 8 – Life cycle analysis (LCA) scheme.

The basis of the software is an attributional life cycle analysis in which several bills of materials are considered as well as the process that allows a vehicle to work. Thus, different fuel production, electricity mixes and components productions can be extracted from the software database. The main environmental impact indicators are: Total Energy, Fossil, Coal, Natural gas, Biomass, Nuclear and Renewable fuels, Water usage as reservoir, irrigation, cooling, mining and process, different pollutant emissions and Land-Use change (LUC). The lifetime of the vehicle was taken as 150,000 km as the average considered for no-hybrid and hybrid electric vehicles without battery replacement [45]. In addition, the evaluation of the emissions during the vehicle use was performed with the results obtained in the OD-numerical model with the WLTC. As this driving cycle was created to represent the daily use for any person around the world, it would be the most representant average cycle.

Other crucial task is the specification of the fuel production location due to the diverse energy matrix of the countries. As the bio-ethanol is already well establish in US and Brazil, this both scenarios were taken as parameter to evaluate the different technologies. Therefore, Table 5 shows the main impact indicators used in the LCA analysis. The table represents for each fuel-source the necessary energy and release CO₂ emissions to produces and transport 1 MJ of the fuel up to the fuel station. The CO₂ due to biogenic source and land use change consider the renewable sources and their effect on the change in carbon stocks between the carbon pools of the terrestrial ecosystem. The total CO₂ considers the sum of these three parameters. It is important to note, that GREET database does not consider the direct and indirect LUC for Brazil ethanol production. However, recent studies [46,47] show the impact of the large-scale ethanol from sugarcane. Therefore, the study performed by Mekonnen et al. [48] was taken as reference for estimated the LUC in US and Brazil. In addition, the GWP-100 indicator adds the effect of other pollutant as CH₄ and N₂O to compare the amount of heat trapped by a certain mass of the gas in question to the amount of heat trapped by a similar mass of carbon dioxide and is expressed as a factor of carbon dioxide (whose

GWP is standardized to 1) over 100 years. For more information about the source of each components could be found in Argon website [49].

Table 5 – Main impact indicators used in the LCA for USA and Brazil estimated by MJ of fuel produced.

Fuel	Energy [MJ]	CO ₂ [g]	CO ₂ Biogenic [g]	CO ₂ Land use change [g]	CO ₂ total [g]	GWP-100 [g]	Information Source
E100 USA	1.68	33.0	0.0	7.4	40.4	52.2	[48,50]
E100 BR	3.35	178.0	-163.4	16.0	30.6	23.4	[48,51]
E85 USA	1.58	29.2	0.0	5.7	34.9	44.7	[48,50]
E85 BR	2.86	140.5	-125.5	13.6	28.6	22.7	[48,51]
H ₂	1.52	85.9	0.0	0.0	85.9	92.8	[52]
Diesel	1.20	13.4	0.0	0.0	13.4	16.7	[53]
Gasoline	1.24	16.7	0.0	0.0	16.7	20.2	
Electricity USA	1.91	117.2	-0.7	0.0	116.5	123.8	[54]
Electricity BR	1.66	57.3	-27.5	0.0	29.8	31.9	[55]

*USA: United States of America, BR: Brazil

It is important to note that the bio-ethanol has a 100% biogenic carbon mass ratio. This means that all CO₂ emission produced in the combustion by the vehicle use are zero at the end of the analysis. CO₂ emissions stemming from the biogenic matter are regarded as carbon neutral, whereas CO₂ from fossil matter is climate-relevant. Other important assumptions are that the vehicle fabrication and components (battery, electric motors, tires, etc) were the same for both scenarios. As the information is complex to be obtained and it is not available in GREET database for each country, the variation of these components is only by size, materials and capacity.

3. Results and discussion

The results are divided into three subsections. The first subsection shows the results of the optimization procedure for the different vehicle platforms to perform the WLTC with the minimum energy consumption. Emissions results are discussed to determine the potential of each combustion mode. In a second subsection, the optimized vehicle platforms are tested in different real-life driving cycle to observe the differences to the observed in the homologation cycle. This procedure allows to study the vehicle concept, 90 kW electric propulsion and 30 kW of range extender capacity, in a more demanding cycle to show the potential for real applications. Finally, the last subsection presents a life cycle analysis with focus in the benefits on the use bio-ethanol as renewable energy to reduce CO₂ emissions in an integrate overall perspective.

3.1. Vehicle Optimization Results

Figure 9 shows the performance global values of the successful cases for each combustion mode in the range extender vehicle through the WLTC. Around 70% of the 800 cases achieved the required final SOC (65%) together with minimum deviation of the cycle speed (± 2 km/h) as required by the WLTP regulation [56]. The baseline case is the no-hybrid propelled by a SI-PFI engine with E100 and stoichiometric air-fuel ratio. Figure 9a shows the total mass consumption against the NO_x engine-out emissions for

each concept. The electrification of the powertrain by this series layout strongly decreases the fuel mass consumption. The SI system with hybrid mode is below the baseline for all the cases tested. Mainly justified by the improvement of the ICE efficiency due to work in stationary points instead of transient conditions and the recovered brake energy along the cycle. For this driving cycle, the lost energy by braking in the no-hybrid vehicle is around 26% of the tractive energy required. As the high traction motor capacity (90 kW), the 95% of the brake energy is recovered and storage in the 400 V battery in this range extender concept. On the other hand, the electrification of the powertrain does not allow an important reduction in NO_x levels. The SI mode in the both powertrain platforms (no-hybrid and range extender) cannot reduce the engine-out NO_x below 1.0 g/km. The Euro 6 normative levels are 0.06-0.08 g/km for PI and CI engines, respectively (see Table 2).

Figure 9 shows that advanced combustion modes allow a strong decrease of the NO_x emissions. The RCCI, thanks to an extreme low NO_x calibration map (Figure 7c), reaches emissions below the maximum regulation levels (dotted vertical line). In spite of the PCIS lean combustion strongly reduction of the NO_x emissions (76%) with respect to the homologous SI system, it is not enough to enter in the legislation levels. The calibration performed for the PCIS with E100-hydrogen needs to be improved in terms of NO_x emissions to avoid an aftertreatment device in the exhaust tailpipe.

Figure 9b shows the energy consumption for the different vehicle platforms. The optimum cases, minimum energy consumption, are depicted in square points for each vehicle platform. As the hydrogen has a higher LHV than bio-ethanol (Table 4), the benefits seen in the mass consumption graph were opposite between SI and PCIS. The SI system achieve a thermal efficiency of 41%, meanwhile the PCIS 37%. The RCCI thermal efficiency (39%) was higher than the PCIS but still lower than the SI. This explains the fact that the SI range extender DoE points are slightly below the other concepts. The baseline (SI no hybrid) achieved a total brake thermal efficiency of 32%. Therefore, the operation in stationary conditions instead of transitions point in the ICE has a positive effect in the combustion efficiency. The extra benefit with respect to the no-hybrid vehicle are associated to the regenerative braking mode as abovementioned.

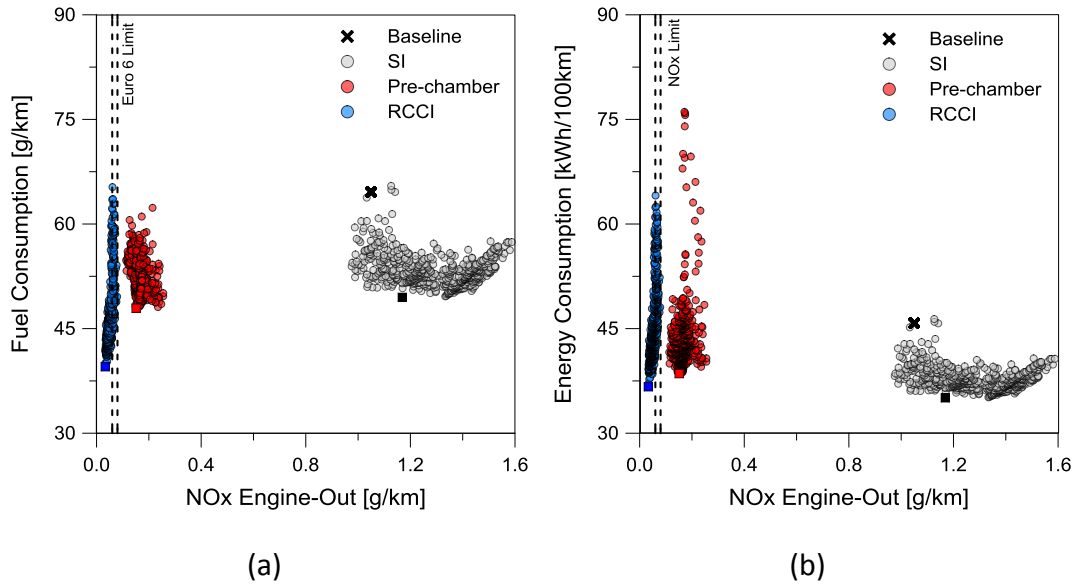


Figure 9 – Total fuel mass consumption (a) and energy consumption (b) against NO_x engine-out for the hybrid DoE cases and the baseline.

Figure 10 shows the two hardware parameters studied in the DoE for the range extender platforms. Figure 10a depicts the effect of the battery size in the energy consumption along the WLTC. The decrease of the battery capacity improves the energy consumption due to lower additional weight. Therefore, the range between 3 and 4 kWh is the best design to allow energy storage without losing excessive energy for additional weight. The gear ratio (Figure 10b) was also optimized to find the best generator rotational speed depending on the engine platform. The higher the gear ratio, the lower generator rotational speed. Despite the effect in the consumption, it is minimum with respect to the operational points selection. The generator has an optimum efficiency between 1000 – 3000 rpm.

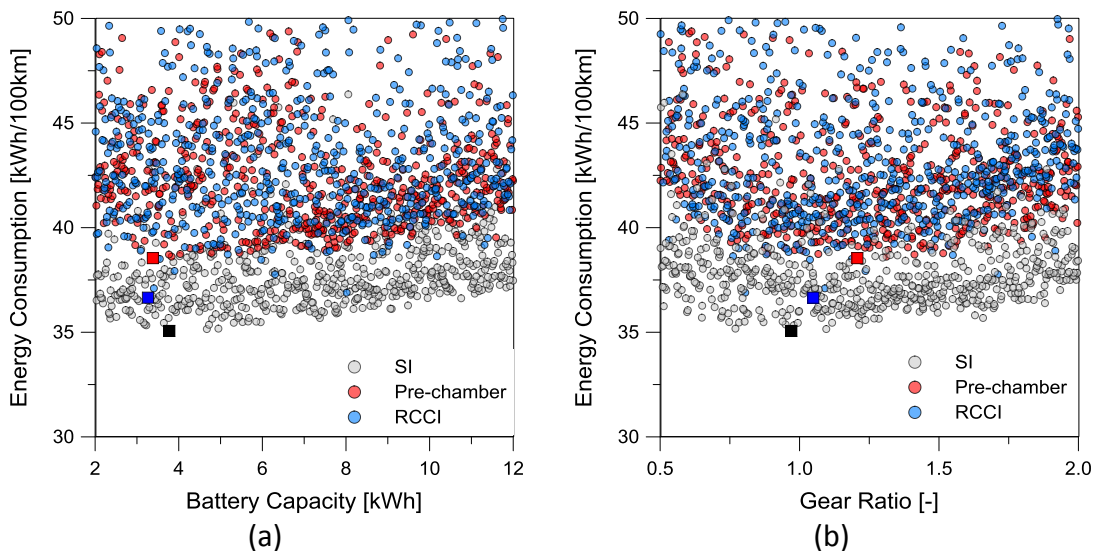


Figure 10 – Energy consumption against battery capacity (a) and gear ratio between ICE-GEN (b) for the range extender platforms.

Although the best powertrain was set up to minimize the energy consumption, one of the main objectives of this work is the reduction of CO₂ and NO_x with respect to the

baseline. Figure 11 shows the effect in the CO₂ when the powertrain was electrified and the combustion mode was altered. The 2021 European target was added in the graph as vertical dashed line for reference. For a SI-PFI engine the range extender allows an average CO₂ emissions reduction of 15% with respect to the baseline. Also, it is possible to achieve the 2021 target selecting a properly operational point. However, the NO_x emissions are far from legislation targets and an ATS is required.

For the advanced combustion modes, two different trends are seen. The PCIS allows a strong reduction of CO₂ with a minimum of 60 g/km (below 2030 target) but the NO_x is above the legislation limits (0.06 g/km). Moreover, these extreme low CO₂ points operate with relatively high amount of hydrogen (35% of the total mass). Therefore, the energy consumption is two times higher than the optimum case. In spite of not achieving 2030 target, the optimum case for the PCIS is below the 2021 target. In case to need extreme low CO₂ emissions, PCIS shows potential to achieve this requirement if energy consumption it is not a main limitation. On the other hand, the RCCI operation is below the NO_x emissions limits but the CO₂ do not decrease as far as the PCIS. The optimum case is 6 g/km over 2021 target. The red dashed box in Figure 11 represents the ideal case in which 2021 CO₂ target and NO_x limits are reached. None of the cases tested in this work can achieve the desired values without an aftertreatment system or advance vehicle technologies to improve total efficiency. This shows the difficulties of car manufacturers and researches to achieve the government requirements. In spite of not achieving the desired target, it is clear that the advanced combustion modes working with bio-ethanol is a potential solution to continue improvement the commercial passenger vehicles to reduce pollutant emissions.

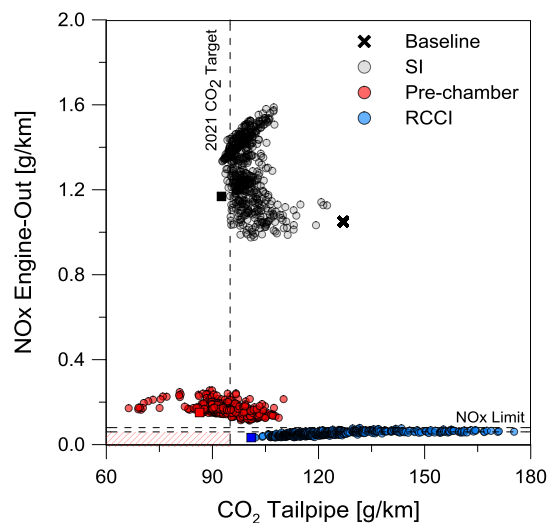


Figure 11 – NO_x engine-out against CO₂ emissions at the tailpipe for the hybrid DoE cases and the baseline.

The particle matter emissions are restricted in vehicle operation due to the well-known harmful effect to the human health. For conventional diesel combustion (CDC) and SI gasoline direct injection (GDI) engines the amount of PM at engine-out are far over the limit [43]. This is the main reason that comply with Euro 6 the vehicle manufacturers use complex aftertreatment systems to reduce particle matter (DPF-Diesel Particle Filter and GPF-Gasoline Particle Filter) below the limits (0.05 g/km). Advanced combustion modes such as RCCI take relevance due to the possibility to reduce PM using homogeneous fuel-air charge and reducing wall impingements that

produce diffusive flames and later soot. On the other hand, it is well known that the use of port fuel injection instead of direct injection in positive ignition engines avoids the production of particle matter. Berndorfer et al. [43] shows that already in Euro 4 engines the PM was below 0.4 mg/km when the gasoline was injected in the intake port. This is the main reason why Euro 6 does not restrict the PM in PFI engines. For this work, only the RCCI mode was evaluated in terms of soot and the other combustion modes were supposed zero.

Figure 12 shows that for the RCCI-Bio-ethanol in the range extender platform is below Euro 6 limits. Therefore, an ATS as a DPF device is not necessary to reduce this component. The main reason of this ultra-low soot is the bio-ethanol injection before the diesel, which creates a homogeneous air-fuel mixture. In addition, the diesel injection is reduced compared with the CDC case. Therefore, the soot levels are below the limit for all cases tested. Additional to the NO_x decrease, the avoid of the creation of soot is the other strong point of this low temperature combustion mode.

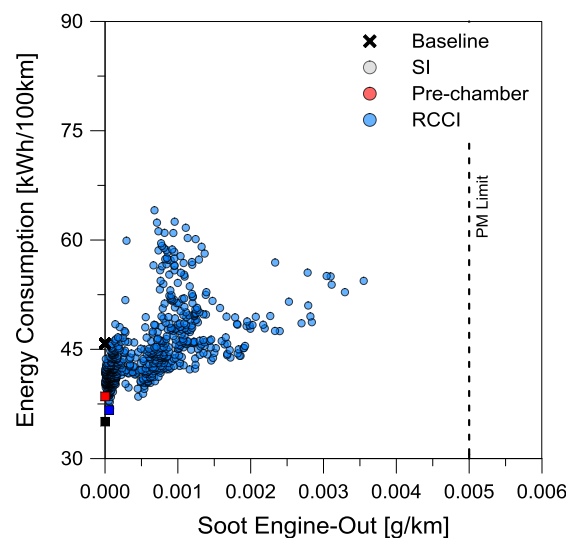


Figure 12 –Energy consumption against particle matter (PM) engine-out for the hybrid DoE cases and the baseline.

The CO and HC are also restricted by the normative. Specifically, SI engines operating with gasoline and bio-ethanol generally presents high amounts of these gases in the exhaust due to partially or not burned fuel. The earlier injection of the air-fuel mixture enhances the effect of trapped fuel in crevice zones. In the RCCI combustion this phenomenon is also expected due to the injection of the low reactivity fuel (gasoline or bio-ethanol) in the intake port [42]. Generally, conventional diesel combustion has minimum CO and HC at engine-out thanks to the lean combustion and the diesel direct injection [57].

Figure 13a shows that the PCIS achieves reduction of CO emissions with respect to the SI cases. The optimum selected case is below the limit (second vertical dashed line). This is mainly by the lean combustion (excess of air) that helps to reduce incomplete combustion. Additionally, the range extender operation helps to reduce CO emissions due to the use of high efficiency engine map zone (high load) in which the combustion is improved. A no-hybrid vehicle during idling and low load zones produce high amount of this harmful component (see baseline and SI-hybrid in Figure 13a). The RCCI produces the largest amount of CO when compared with the other combustion modes in most of the cases tested. However, for a certain range in which the combustion efficiency is high

(low energy requirements) the CO emissions are closer to SI combustion or lower. The Euro 6 establishes 0.5 g/km (first dashed line) for CI ICE. Therefore, a catalyzer is necessary to reduce this emission component. The main reasons are the not burned fuel trapped in the crevices. This effect is expected due to the above-mentioned effects and previously seen in the bibliography in LTC modes in CI engines [58]. In spite of having cases with more than 8 g/km of CO at engine-out, the optimum case is as much as the SI-hybrid and below the baseline.

Figure 13b shows similar effect with the engine-out HC emissions. The RCCI is again the largest in terms of this component emissions along the cycle. The main difference with the previous analyzed graph is the emissions measured in the PCIS that are higher than in the SI mode. This can be attributed to crevice addition with the pre-chamber and low combustion temperature, typically of lean combustion. Also, misfire events observed in the higher combustion variability (CoV_{IMEP}) than the SI stoichiometric case. Although, the PCIS CoV_{IMEP} was controlled to be below 5% to ensure vehicle drivability, the SI was never above 3%. Despite the trends analyzed, all of the cases are above the limit. This means that an ATS system like TWC for the stoichiometric SI cases or a specially designed catalyzt to reduce these components (CO and HC) is necessary.

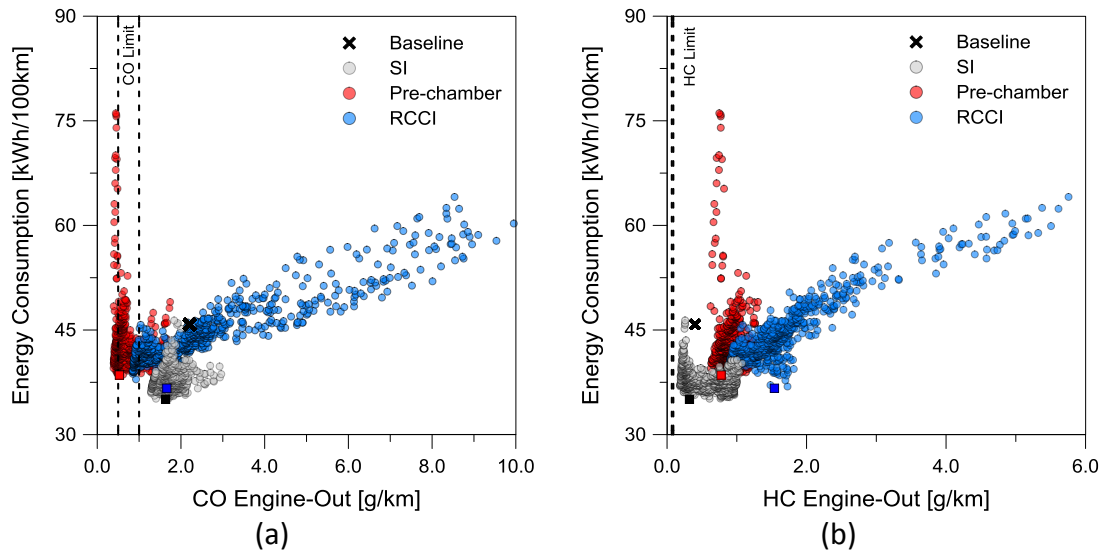


Figure 13 – Energy consumption against CO (a) and HC (b) engine-out for the hybrid DoE cases and the baseline.

Table 6 shows a resume of the optimum vehicle platforms set up to achieve the minimum fuel consumption in a WLTC. The main performance parameters as fuel consumption and emissions are also included. In addition, it was included the necessary fuel tank capacity to achieve the same fuel autonomy of the baseline (580 km). The range extender could decrease in around 10 lt the fuel tank. This would lead more fuel economy benefits due to the decrease of total vehicle weight. In the case of the dual fuel platforms (RCCI and PCIS), the results show that it is not necessary to increase the fuel tank. The RCCI could be solved with a division of the OEM tank in two with 80% for bio-ethanol and 20% for diesel. The PCIS will use a similar bio-ethanol tank capacity to the SI-Range extender but a H₂ tank of 1.0 kg capacity needs to be added. In this case a pressure of storage was set in 700 bar (density of 30 g/lt), which is commonly used in commercial hydrogen and fuel cell vehicles [59]. In spite of being low weight of additional fuel, it will induce to another type of fuel tank (high-pressure) with large

volume capacity (similar to the bio-ethanol tank). Therefore, it is the most complicated in terms of fuel storage system.

Table 6 – Optimum hardware and control set up for the different vehicle platforms.

Parameter	No-Hybrid	Series HEV		
	SI	SI	PCIS	RCCI
Battery Capacity [kWh]	-	3.0	2.9	5.1
Operation point [kW]/[rpm]	-	29/2960	27/3000	20/2080
Vehicle Mass [kg]	1145	1185	1181	1180
Energy Consumption [kWh/100km]	45.8	35.1	38.5	36.7
Bio-ethanol (E100 or E85) volume consumption [lt/100km]	8.1	6.2	5.8	4.2
Diesel or H ₂ volume consumption [lt/100km]	-	-	5.8	0.8
NO _x Engine-Out [g/km]	1.05	1.17	0.15	0.03
CO ₂ Tailpipe [g/km]	121	93	86	101
Bio-ethanol Tank _{@580km} [lt]	47	36	34	24
Diesel Tank _{@580km} [lt]	-	-	-	5
H ₂ Tank _{@580km} [lt-kg]	-	-	34 - 1.0	-

3.2. Real Life Driving Cycles Results

The optimized range extender vehicles were tested in three real driving cycles in order to represent urban, urban-rural and highway driving cycles. This section intends to show the potential of the previous designed concepts and the limitations when are used in driving cycles different than the homologation. To achieve the same SOC level that at the beginning of the cycle (65%), the batteries were recharged up to 2 minutes after the end of the cycle. This condition represents a real situation in which the cycle suddenly stops, and the vehicle is put into parking mode.

Figure 14 show the CO₂ emissions and engine-out NO_x emissions along the urban cycle (Figure 4b). There is a strong reduction in CO₂ emissions of all range extender concepts with respect to the baseline (no-hybrid). This is mainly due to two reasons: 1) In urban cycles the no-hybrid concept has a decrease in ICE thermal efficiency and 2) The regenerative braking available in urban cycles is higher than in the WLTC due to more stop events. For this case, the hybrid concepts maintain the ICE efficiency around 38%, unlike the no-hybrid, which presented a decrease of 19% with respect to the homologation cycle (WLTC). In addition, the not recovered brake energy in the baseline (no-hybrid) case represents 70% of the tractive energy. This energy it is almost completely recover in the range extender cases (90%). The PCIS has the lowest CO₂ emissions due to the combination of a high efficiency engine operating with a low carbon fuel (E100) and zero carbon fuel (H₂). The RCCI has the highest CO₂ emissions between the hybrid concepts due to the higher E85 and Diesel carbon content. On the other hand, the NO_x emission was the lowest and below the Euro 6 requirements for this concept.

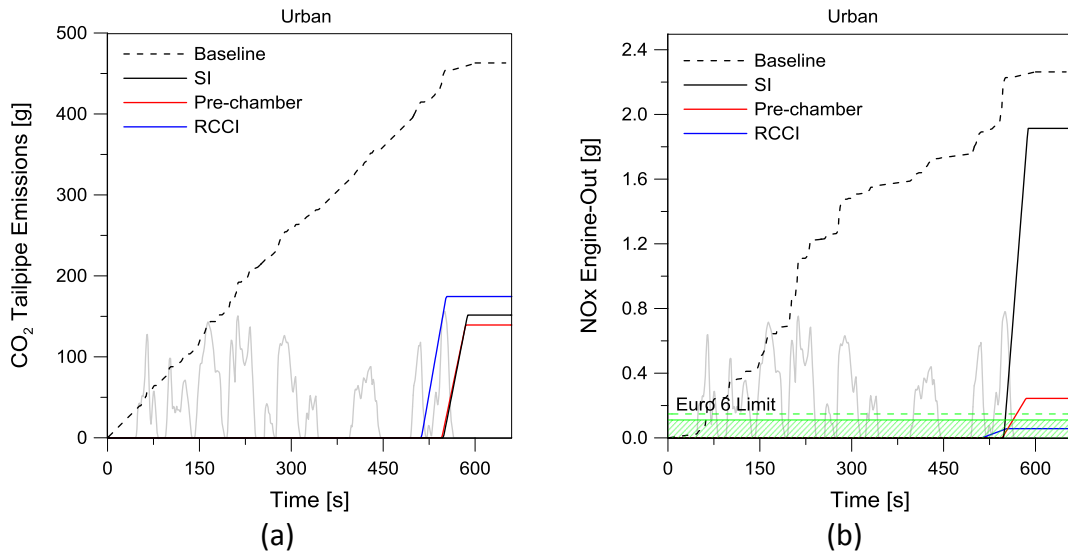


Figure 14 – CO₂ at the tailpipe (a) and NO_x engine-out emissions (b) for the urban real driving cycle under different range extender platforms and baseline case.

Figure 15 shows the results for a combined (Urban + Rural) cycle for all vehicle platforms. The benefits in CO₂ emissions are lower than a similar combined cycle as the WLTC (Figure 15a). For this case, the hybridization of the vehicle presented no improvements for the RCCI mode and low benefits for the SI and PCIS. The main explanation for this behavior is the low regenerative braking available (7% of the tractive energy). Also, the hybrid concepts use the level 2 of charge (maximum power) due to harder conditions than the WLTC. This would lead to higher mechanical losses, mainly in the generator by change the operational point. On the other hand, Figure 15b shows that the use of advanced combustion modes (RCCI and PCIS) allows a strong reduction of NO_x. Due to the RCCI ultra-low NO_x calibration, the final emissions are below Euro 6 limits.

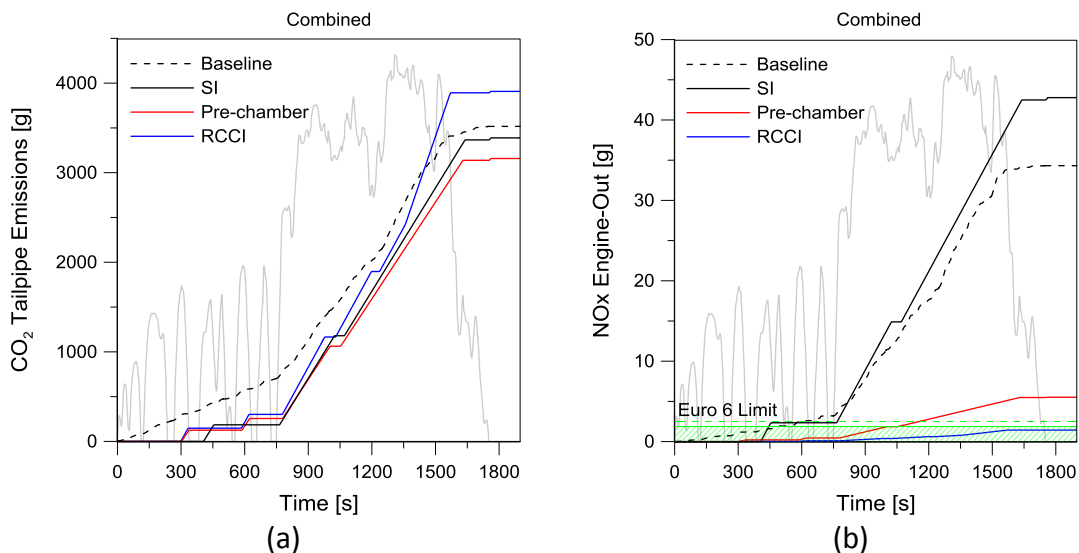


Figure 15 – CO₂ at the tailpipe (a) and NO_x engine-out emissions (b) for the combined real driving cycle under different range extender platforms and baseline case.

The last cycle tested was the highway, which contains around 260 km of practically constant speed (120 km/h). The cycle starts from stop position and ends after reducing the speed from 125 km/h to zero. The main idea of this test is to understand if it is

possible to promote a long travel with a concept that only has an ICE of 30 kW to operate as range extender. In addition, the study of the final performance values was conducted to evaluate its benefits when compared to a conventional vehicle. Figure 16a shows that the baseline working as no-hybrid with E100 has the lowest CO₂ emissions. Also, Table 7 shows that it has the lowest energy consumption. This is mainly justified as the highway the ICE operates with similar high efficiency as in range extender mode but the mechanical losses are lower (55%). The PCIS has achieved similar CO₂ emissions to the baseline due to the H₂ content in the fuel burned. However, the energy consumption is similar to the RCCI concept. The NO_x emissions (Figure 16b) are strongly lower for advanced combustion modes than the SI-PFI concept. The RCCI due to the ultra-low NO_x calibration can achieve the Euro 6 limit also in a high-demand highway cycle.

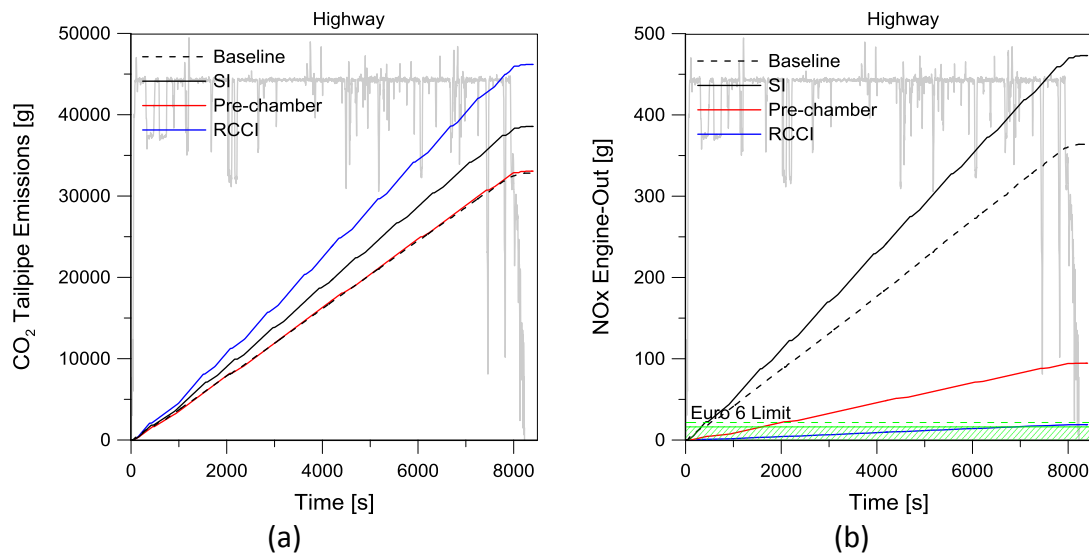


Figure 16 – CO₂ at the tailpipe (a) and NO_x engine-out emissions (b) for the highway real driving cycle under different range extender platforms and baseline case.

Table 7 contains all the information with respect to the performance and emission for the three-driving cycle tested. In general, the range extender concept shows great advantage in urban cycles in which the brake energy recovery is above the 50% of the traction required energy. In addition, the ICE operates with higher efficiency than in a no-hybrid concept due to the avoid of using low loads and idle mode. In combined cycles, the benefits depend on the ratio between urban and rural areas being the homologation cycle better than the real combined cycle tested for hybrid concepts. Lastly, at highway conditions the range extender shows decrement in the total vehicle efficiency as well as low benefits in CO₂ emissions.

In terms of NO_x emissions, the use of advance combustion modes leads in a strong reduction of engine-out. RCCI operating with bio-ethanol and diesel can achieve Euro 6 level for all the cycles tested. Therefore, ATS is not necessary for this concept car (RCCI + Range Extender). For the PCIS, the NO_x levels are low but still over the emission regulation. Therefore, an ATS like NO_x lean tramp [60] or similar technology could be enough to achieve Euro 6 level (0.06 g/km). In the case of SI-PFI no-hybrid and range extender the NO_x emissions are far above of the limits. However, for this type of concepts a TWC can be used due to the stoichiometric operation. For the range extender operation additional tests need to be conducted to know if a traditional TWC developed for conventional vehicles can be used. As it is well known the TWC has a minimum

temperature of operation (light off temperature) to be effective to reduce the NO_x. As the hybrid start and stop the ICE several times, problems with emissions can appear. In this sense, the PCIS or RCCI has more advantage to control emissions.

Table 7 – PCIS and RCCI hybrid vehicles in real life driving cycles.

Driving Cycle	Parameter	No-Hybrid	Series HEV		
		SI	SI	PCIS	RCCI
Urban	Energy Consumption [kWh/100km]	96.3	31.0	34.3	34.2
	Bio-ethanol (E100 or E85) volume consumption [lt/100km]	17.0	5.5	5.0	3.9
	Diesel or H ₂ volume consumption [lt/100km]	-	-	5.8	0.7
	NO _x engine-Out [g/km]	1.24	1.03	0.13	0.03
	CO ₂ Tailpipe [g/km]	254	82	75	94
Combined	Energy Consumption [kWh/100km]	42.8	41.1	44.8	45.5
	Bio-ethanol (E100 or E85) volume consumption [lt/100km]	7.6	7.3	6.8	4.9
	Diesel or H ₂ volume consumption [lt/100km]	-	-	6.5	1.2
	NO _x engine-Out [g/km]	1.10	1.37	0.18	0.05
	CO ₂ Tailpipe [g/km]	113	113	101	126
Highway	Energy Consumption [kWh/100km]	46.3	54.2	63.7	62.4
	Bio-ethanol (E100 or E85) volume consumption [lt/100km]	8.2	9.6	8.2	6.2
	Diesel or H ₂ volume consumption [lt/100km]	-	-	17.2	2.0
	NO _x engine-Out [g/km]	1.35	1.75	0.35	0.07
	CO ₂ Tailpipe [g/km]	122	143	123	171

3.3. Life Cycle Analysis Results

The LCA results are presented in this section using the GREET database (version 13520, GREET 2019, Argonne Laboratory) for two different scenarios. US and Brazil were studied as bio-ethanol is well established as commercial fuel in these countries and the well to tank (WTT) information are well known. To complement the four cases model in the previous section, an electric vehicle and two SI gasoline platforms were added. The first case was simulated using GT-Suite with the same methodology than the range extender platforms. The battery capacity was increased (36 kWh) but with the same nominal voltage (400 V). The maximum power output was set at 90 kW as the other vehicles. On the other hand, to estimate the CO₂ and energy consumption for the SI gasoline no-hybrid vehicle, the 2018 and 2021 EU vehicle references were used. This means that the 120 g/km and 95 g/km values were taken to the LCA analysis. The energy consumption was calculated with the assumption of stoichiometric ideal combustion.

Figure 17 shows the LCA CO₂ emissions for the different vehicle platforms using fuels produced in the US. The left bar graph shows the CO₂ emissions without considering the biogenic indicator and land use change effect. The gasoline 2021 concept (TTW 120 g/km) and the battery electric vehicle shows the lowest values. The gasoline vehicle combines low tailpipe emission together with a lower cost in terms of CO₂ to produce

the gasoline instead of the bio-ethanol (orange bar). Also, battery and electricity production emissions are lower than the WTW for bio-ethanol vehicles.

However, when considering the biogenic effect and land use change of the bio-ethanol, the trend is reverted (Figure 17b). All platforms using E100 or E85 results in lower total LCA CO₂ emissions than BEV or gasoline concepts. The biogenic effect neglects the tailpipe CO₂ emissions and is stronger than the land use change effect. Therefore, the fuel and vehicle production are the parameters that have effect in the total result. The range extender SI E100 is the best case, followed by the SI no-hybrid. The PCIS was 4% higher due to the hydrogen production CO₂ emissions. In the case of the RCCI, it is 26% higher due to the no-biogenic property of the diesel.

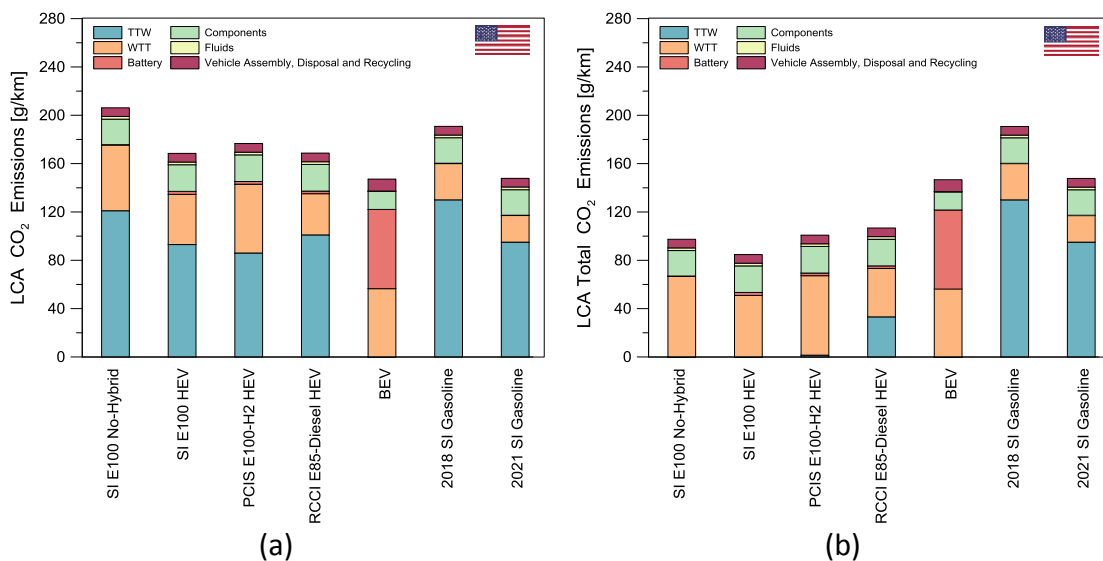


Figure 17 – LCA CO₂ emissions in US scenario not considering (a) and considering (b) the biogenic indicator and land use change effect.

Figure 18 shows a similar analysis but using the fuel production in Brazil. The CO₂ cost to produce the bio-ethanol from sugarcane is five times higher than in US (see Table 5). Also, the renewable source of the electricity in Brazil (mainly hydroelectric) leads to high gains in the use of BEV than bio-ethanol propelled vehicles when looking in the LCA CO₂ direct emissions. In addition, the gasoline vehicles result shows improvements with respect to the baseline. However, adding the biogenic effect in the use and production of the bio-ethanol, the CO₂ has a strong decrease. Similar trend to what is seen for US (Figure 17b) is depicted in Figure 18b. The main difference in these two countries is the higher benefits of using electric vehicles than gasoline due to the renewable source. In spite the LUC of Brazil is two times US impact, the ethanol fueled vehicles still being cleaner than gasoline and battery electric vehicles. The RCCI E85-Diesel was the highest in the ethanol fueled vehicles due to the Diesel (HRF) and gasoline (E85) use. These two fuels not contain the CO₂ reduction due to biogenic effect.

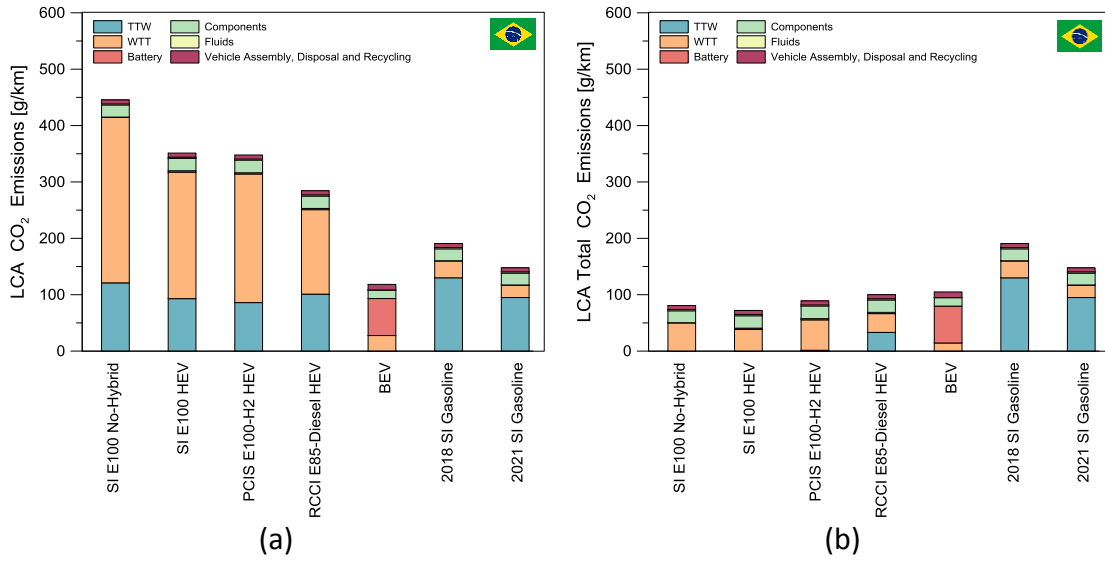


Figure 18 – LCA CO₂ emissions in Brazil scenario not considering (a) and considering (b) the biogenic indicator and land use change effect.

To resume the results in both scenarios, Figure 19 shows the GHG in a period of 100 years. To summarize the results in both scenarios, Figure 19 shows the GWP in a period of 100 years. GWP-100 takes into account the total CO₂ results together with the effect of other pollutant emissions as methane and nitrous oxides. In general, the same trend is seen for both countries, with gasoline concepts achieving the highest values. Although BEV has zero tailpipe emissions, the bio-ethanol vehicles contribute to lower CO₂ emissions than this technology. In this sense, the bio-ethanol shows benefits to reduce the global air pollution in both scenarios.

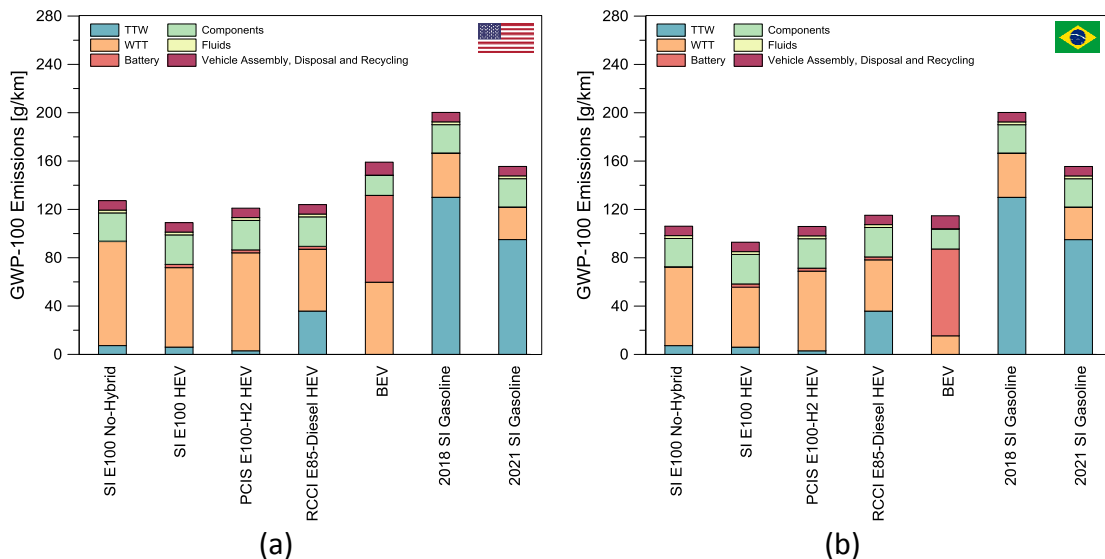


Figure 19 – Global warming potentials (GWP) over 100 years in US (a) and Brazil (b) for different vehicle platforms.

4. Conclusions

This work has investigated the benefits of using advanced combustion modes and hybrid electric technology in vehicles fueled with bio-ethanol to achieve governmental emissions targets. This means to achieve simultaneously Euro 6 NO_x and soot emissions levels together with the CO₂ 2021 target (95 g/km). The results obtained by means of a map based OD vehicle model were used to compare the potential of two advanced combustion concepts in hybrid powertrains. A conventional SI-no hybrid bio-ethanol vehicle representative of commercial class B vehicles was used as baseline. Different homologation and real-life driving cycles were tested. The GHG emissions were analyzed in different levels, from TTW to LCA view. The main results can be summarized as follows:

- General results:
 - It is possible to equip a class B vehicle with a de-rated ICE operating under advanced combustion concepts fueled with bio-ethanol.
 - The range extender concepts presented in the work show acceptable performance in homologation and real-life driving cycles with top speed over 130 km/h and highway cycles with over 200 km of extension.
 - The battery capacity was not a critical parameter in the optimization with an optimum value of 3.5 kWh for all the range extender concepts.
 - The fuel tank for the dual fuel concepts was estimated to achieve the same autonomy range than the baseline vehicle. It was found that no additional space was necessary in the OEM vehicle, but only slight modifications to carry on two different fuels.
 - In spite of these improvements in terms NO_x and GHG emissions of the advanced combustion modes, more work needs to be done to stablish these technologies in large scale.
- Tank to Wheel results:
 - The PCIS operating as range extender can achieve ultra-low CO₂ emissions. A minimum of 60 g/km of CO₂ was achieved with an operational point of high H₂ mass rate. However, the energy consumption increases by 2 times with respect to the baseline (SI E100).
 - When selecting an ICE operational point of low H₂ mass injected for the PCIS, similar energy consumption than the baseline case is achieved. Moreover, the NO_x emissions are reduced up to 7 times. Also, the 2021 CO₂ target is achieved with 7 g/km lower than the SI E100 in the current European homologation cycle (WLTC).
 - The RCCI has the highest gains in terms of energy consumption and NO_x reduction with respect to the baseline case. In addition, it is possible to achieve Euro 6 NO_x and soot levels in the WLTC with the RCCI bio-ethanol range extender vehicle.
 - In spite of achieving the best energy consumption results, the CO₂ emissions for RCCI are over the 2021 CO₂ target due to the higher Diesel and E85 carbon ratio than the E100.

- The results in real life driving cycles were significantly different than for the WLTC. In this sense, the urban case shows great improvements for the hybrid range extender vehicles, with CO₂ and NO_x gains of 3 and 9 times for the advanced combustion modes, respectively. Contrarily, in the highway cycle the hybrid concepts do not show improvements over the conventional powertrain due to excessive mechanical and battery losses.
- LCA results:
 - The bio-ethanol propelled vehicle in hybrid and no-hybrid powertrains shows better gains in GHG emission than pure battery electric and gasoline 2018 and 2021 vehicles in both country scenarios.
 - The LCA shows a similar trend for US and Brazil but with a decrease of GWP-100 for all concepts in Brazil due to a more renewable energy mix. This is mainly due to the biogenic fuel production of bio-ethanol that compensates the higher CO₂ fuel production and land-use-change for compared with US.
 - The biogenic indicator of the bio-ethanol allows to achieve ultra-low TTW emissions. This compensates the higher WTT of the bio-ethanol with respect to the gasoline production and the battery production included in the hybrid vehicles. Therefore, the LCA shows that the use of bio-ethanol allows to achieve lower GWP-100 emissions than an efficient gasoline vehicle (2021 vehicle concept).
 - The comparison with respect to a BEV shows that, despite the zero TTW emissions and reduced TTW emissions due to the electricity mix, the high capacity battery size required to propel the pure electric vehicle induces a higher GWP 100 emissions than the bio-ethanol concepts.
 - In spite of the better results in terms of TTW (CO₂ and NO_x) with the advanced combustion modes, the LCA results show that the higher TTW GHG emissions production of diesel and hydrogen makes that the cleanest concept is the range extender SI bio-ethanol vehicle.

Acknowledgments

The authors acknowledge FEDER, CAPES and Spanish Ministerio de Economía y Competitividad for partially supporting this research through TRANCO project (TRA2017-87694-R). The authors also acknowledge the Universitat Politècnica de València for partially supporting this research through Convocatoria de ayudas a Primeros Proyectos de Investigación (SP20180148) and the Post-Graduation Program in Mechanical Engineering at UFMG-Brazil for the support provided.

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Abbreviations

1GE	First ethanol generation	GWP-100	Global warming potential over 100 years
2GE	Second ethanol generation	HEV	Hybrid electric vehicle
3GE	Third ethanol generation	HRF	High reactivity fuel
ATS	Aftertreatment systems	ICE	Internal combustion engine
BEV	Battery electric vehicles	IMEP	Indicated mean effective pressure
BMEP	Brake mean effective pressure	LCA	Life cycle analysis
BMEP	Brake mean effective pressure	LHV	Lower heating value
BSCO	Brake specific CO emissions	Li-Ion	Lithium Ion batteries
BSCO ₂	Brake specific CO ₂ emissions	LRF	Low reactivity fuel
BSFC	Brake specific fuel consumption	LTC	Low Temperature Combustion

BSHC	Brake specific HC emissions	OEM	Original equipment manufacturer
BSNOx	Brake specific NOx emissions	PCIS	Pre-chamber ignition system
BSSoot	Brake specific soot emissions	PFI	Port fuel injection
CDC	Conventional diesel combustion	PM	particle matter
CI	Compression Ignition	PN	Particle number
CR	Compression ratio	RBC	Rule based controller
DI	Direct Injection	RCCI	Reactivity Controlled Compression Ignition
DISI	Direct Injection Spark Ignition Engine	rpm	Revolution per minute
DoE	Design of Experiments	SI	Spark Ignition
DPF	Diesel particulate filter	SOC	State of the charge of the battery
E100	96% Ethanol, 4% water	SOI	Start of injection
E85	85% Ethanol, 15% gasoline	TM	Traction Motor
ECU	Engine control unit	TTW	Tank to wheel
EGR	Exhaust gas recirculation	TWC	Three way catalytic
EM	Electric motor	WLTC	Worldwide Harmonized Light Vehicles Cycle
GEN	Generator Motor	WLTP	Worldwide Harmonized Light Test Procedure
GHG	Greenhouse gas emissions	WTW	Well to wheel
GPF	Gasoline particulate filter	λ	Air-Fuel ratio
GREET	Greenhouse gas, Regulated Emissions, and Energy use in Transportation software		

Appendix A

Brake thermal efficiency for the three combustion modes tested in Engine 1 and Engine 2 is depicted in Figure A1. In spite the PCIS uses lower bio-ethanol mass than the SI, the high LHV of the bio-ethanol decrease the final brake efficiency. For the case of RCCI, the maximum brake thermal efficiency is lower than the SI case due to operate in the low-medium load range. Engine 2 can achieve 22 bars of maximum bmep in CDC mode. To improve the thermal efficiency of the RCCI E85-Diesel mode, additional engine modification needs to be done as change the compression ratio and air-exhaust system. In spite of this disadvantage of the advanced combustion modes, the overall efficiency is close to the SI when operates at stationary points.

Figure A2 shows the CO₂ emissions calculated from the mass consumption. This are equivalent to the tailpipe or TTW CO₂ emissions due to the conversion of CO in the aftertreatment device. The best values are for the PCIS due to the H₂ carbon neutral and the E100 low carbon content. Lastly, at Figure A3 the reduction of Soot emission can be seen between RCCI and CDC combustion modes using Engine 2. In spite the CDC was not used along the work, it was added in this section to the reader understand the benefits with respect the conventional mode.

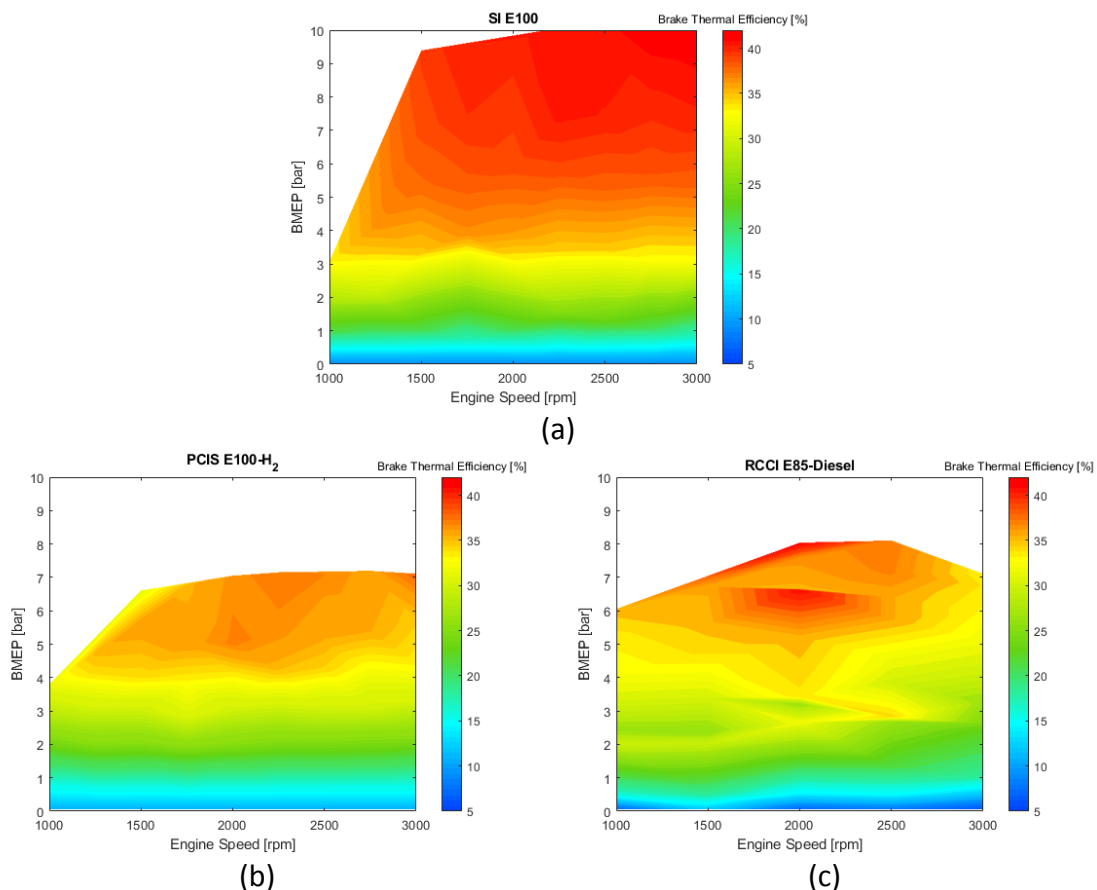


Figure A1 – Brake thermal efficiency for SI E100 (a), PCIS E100-H₂ (b) and RCCI E85-Diesel (c).

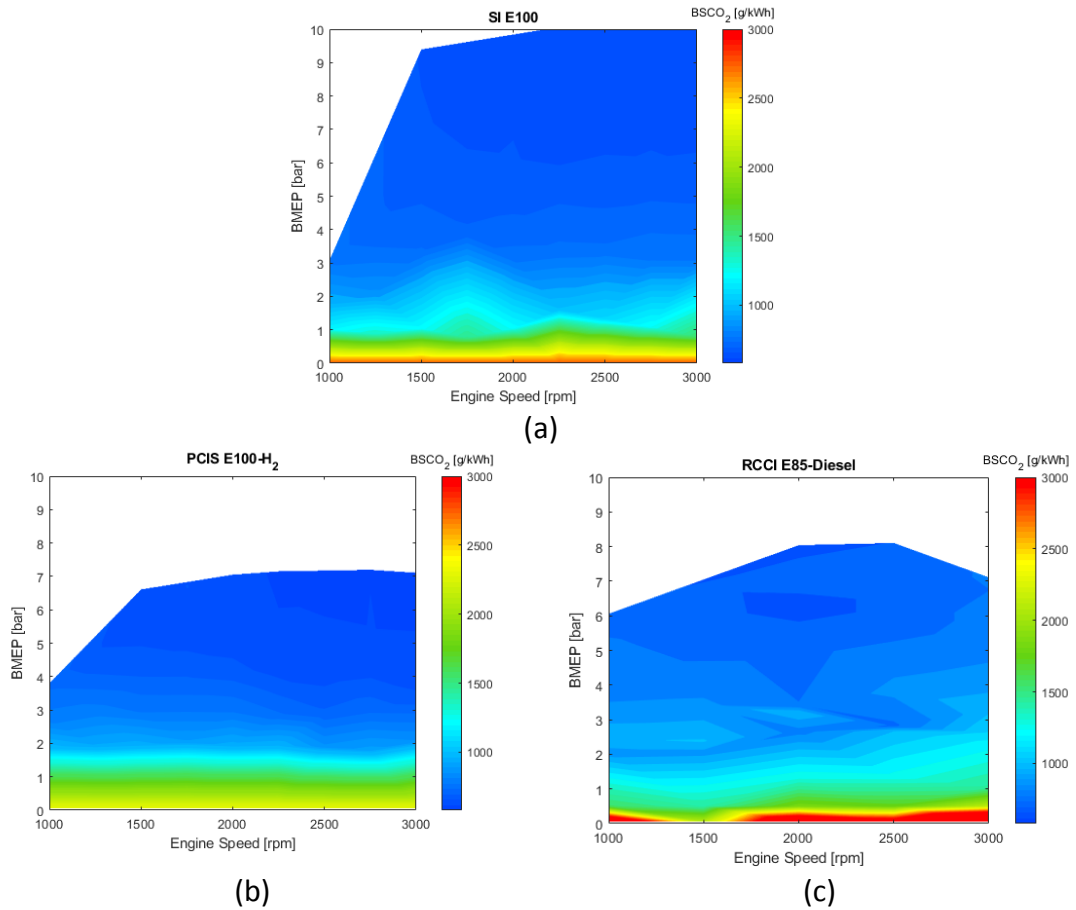


Figure A2 – Brake specific CO₂ emissions at tailpipe for SI E100 (a), PCIS E100-H₂ (b) and RCCI E85-Diesel (c).

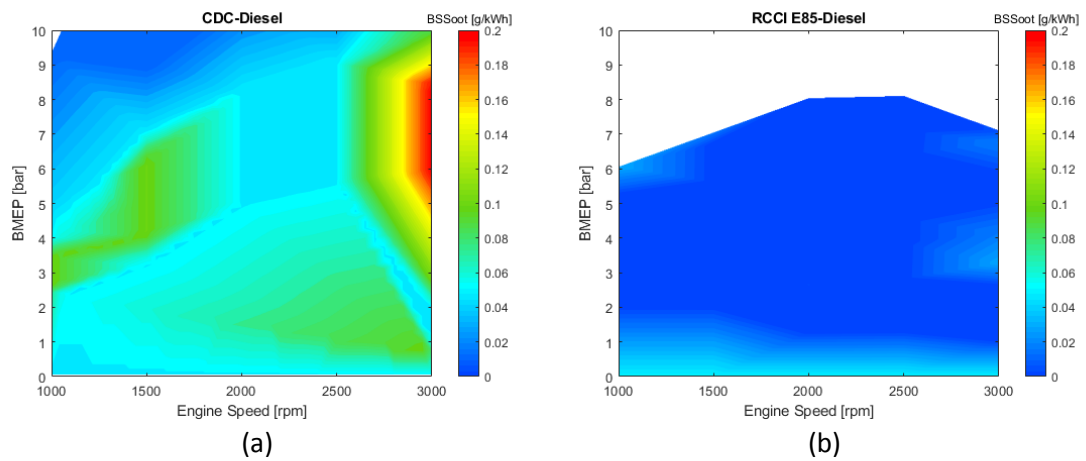


Figure A3 – Brake specific Soot emissions at engine-out CDC-diesel (a) and RCCI E85-Diesel (b) with Engine 2 set up.